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(54) **DESIGN OF COMBINATORIAL MATERIAL LIBRARIES**

ENTWURF VON KOMBINATORISCHEN MATERIALBIBLIOTHEKEN

CONCEPTION DE BIBLIOTHEQUES COMBINATOIRES DE SUBSTANCES

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## Description

### BACKGROUND OF THE INVENTION

**[0001]** The present invention relates to the computer-implemented design of combinatorial libraries of materials. Traditionally, the discovery and development of materials has predominantly been a trial and error process carried out by scientists who generate data one experiment at a time. This process suffers from low success rates, long time lines, and high costs, particularly as the desired materials increase in complexity. When a material is composed of multiple components, theory provides little guidance, and the large variety of possible combinations of components takes a large amount of time to prepare and analyze.

**[0002]** Combinatorial materials science addresses some of these challenges. Combinatorial materials science refers generally to methods for creating collections or libraries of chemically diverse compounds or materials and/or to methods for rapidly testing or screening these libraries for compounds or materials having desirable performance characteristics and properties. By parallel or rapid serial testing of many compounds or materials, combinatorial techniques accelerate the speed of research, facilitate breakthroughs, and expand the amount of information available to researchers.

**[0003]** Furthermore, the ability to observe the relationships between hundreds or thousands of materials in a short period of time enables scientists to make well-informed decisions in the discovery process and to find unexpected trends.

**[0004]** Researchers employing combinatorial techniques design libraries or arrays containing multiple combinations of starting chemicals. It is desirable to design such libraries to explore a desired phase space of starting components and realize good experimental results at a reasonable cost and period of time. Computer programs have been used for life science libraries, and some software applications have been applied to materials. Many of these programs allow for step-by-step input of a detailed protocol for synthesizing a library of materials, but do not allow for definition of chemical ratios or process parameters. To implement such protocols, the user must manually determine the proper concentration and quantity of each starting material to achieve a desired ratio of starting materials in each library member. For large libraries with shared starting solutions, this becomes unwieldy to solve manually without significantly limiting the diversity studied within one library. Other programs allow for definition of chemical ratios or process parameters to apply to a whole library, by do not provide for high level definition of multi-dimensional variation of these ratios or parameters across the spatial dimensions of the library, also limiting the diversity that may be studied within a single library. Thus, for example, WO 98/15825 shows software programs that allow a user to define a combinatorial synthesis by specifying a number of experimental steps to be applied using a set of predefined chemical building blocks, without permitting the user to define spatial variation of chemical ratios or process parameters at a high level across a library. Some of these programs have been either spreadsheet based or graphic-based. Spreadsheet-like interfaces are, for many users, non-intuitive and difficult to learn. Graphic-based interfaces are somewhat more intuitive, but are limited to supplying direct machine instructions to move volumes of liquid on a specific robotic system. Such interfaces fail to provide the comprehensive conceptual library design assistance that materials discovery chemists would find greatly beneficial. Many existing programs are limited to specific chemistries, such as those used in the pharmaceutical industry, and can only interface with a specific type of synthesis instrument.

### SUMMARY OF THE INVENTION

**[0005]** The invention provides a computer implemented methods according to claim 1 and a computer program product according to claims 26. An embodiment provides a graphical user interface through which the user designs a library conceptually, with the ability to specify the desired material composition of multiple library members in terms of a variety of interrelationships between component materials, such as multiple interdependent gradients or ratios of component materials. The resulting conceptual library design is not constrained by the physical limitations of available library substrates or equipment. The graphical interface allows the user to define variation of chemical ratios or process parameters across a library or across one or more distinct, partially intersecting or completely overlapping sub-regions of the library. The invention receives the user's conceptual design and performs the detailed calculations necessary to determine the precise composition of each member of the library. The invention outputs a data file in a format suitable for manual library preparation or automated preparation using conventional material handling apparatus. The output may include a list of mappings to be performed in preparing a library.

**[0006]** In general, the invention features a computer-implemented method for generating a library design for a combinatorial library of materials. The method includes defining one or more sources and one or more destinations, receiving an input defining a first mapping, using the first mapping to calculate a composition of one or materials assigned to one or more of cells of the destination, and generating a data file defining the library design. Each source is electronic data representing a component to be used in preparing the combinatorial library. Each destination is electronic data

representing an arrangement of cells. The first mapping is electronic data defining a distribution pattern for assigning a component to cells in the arrangement. The distribution pattern includes a minimum and a maximum amount of the component to be assigned to any cell of the arrangement and a gradient to be applied between the minimum and maximum amounts of the component across the cells. The data file includes electronic data representing the sources, the destinations and the mapping.

**[0007]** Implementations of the invention can include one or more of the following advantageous features. The method includes displaying a representation of the library design graphically describing the composition of one or more materials assigned to one or more of the cells. The data file includes electronic data representing one or more sets of properties, each set of properties being associated with one of the sources, the destinations or the mapping. Defining the sources and destinations includes receiving an input from a graphical input device. The input defining a first mapping includes a selection from a set of available mapping types, including a one to one mapping of a component from a source to a cell in the arrangement and a one to many mapping of a component from a source to a plurality of cells in the arrangement. The set of available mapping types also includes a many to many mapping of a plurality of components from a plurality of sources to a plurality of cells in the arrangement, a many to one mapping of a plurality of components from a plurality of sources to a cell in the arrangement. or a set of one or more user-defined equations. The gradient is selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression. The set of properties associated with the mapping includes a source name, a source geometry, a destination name, a destination geometry, a gradient type, and a set of gradient parameters defining the gradient. The method includes receiving an input defining a second mapping, and using the first and second mappings to calculate a composition of one or more materials assigned to one or more of the cells. The second mapping is electronic data defining a second distribution pattern for distributing a second component to cells in the arrangement. The second distribution pattern includes electronic data identifying a fixed amount of the second component to be assigned to one or more cells in the arrangement. The second distribution pattern includes electronic data identifying a minimum and a maximum amount of the second component to be assigned to any of the cells of the arrangement and a second gradient to be applied between the minimum and maximum amounts of the second component across the cells. The method includes generating a modified library design by receiving an input redefining a source, a destination or a mapping, recalculating the composition of one or more materials assigned to one or more of the cells; and generating a data file defining the modified library design. The method includes receiving an input defining one or more parameters, and the data file includes electronic data representing the one or more parameters. Each parameter is electronic data corresponding to a process parameter and defines a parameter value for one or more cells of the arrangement. The parameter values vary between a minimum and a maximum amount. The arrangement comprises two or more cells, ten or more cells, or about ninety-six or more cells.

**[0008]** In an embodiment of the invention the method includes receiving an input defining one or more parameters, and generating a data file defining the library design. Each parameter is electronic data corresponding to a process parameter and defining a parameter value for one or more cells of the arrangement. The parameter value varies between a minimum and a maximum amount. The data file includes electronic data describing the source elements, the destination elements, the mappings and the parameters

**[0009]** Implementations of the invention can include one or more of the following advantageous features. The parameter value is defined to vary over time, across two or more cells in the arrangement, or over time and across two or more cells in the arrangement The parameter value varies according to a gradient selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression. The parameter value corresponds to a process parameter selected from the group consisting of temperature, pressure, time, flow rate and stirring speed.

**[0010]** In another embodiment, the invention features a computer-implemented method for preparing a combinatorial library of materials on a substrate. The method includes creating a library design by defining a set of design elements, generating a data file comprising electronic data describing the set of design elements, and using the data file to cause an automated material handling apparatus to assemble the combinatorial library on a substrate. The set of design elements includes one or more sources representing components to be used in preparing the combinatorial library, one or more destinations, each of which includes an arrangement of one or more cells, and one or more elements selected from the group consisting of a mapping defining a scheme for assigning one or more amounts of a component to one or more cells of an arrangement and a parameter corresponding to a process parameter. The parameter defines a parameter value for one or more cells of the arrangement. The parameter value varies between a minimum and a maximum amount.

**[0011]** In another embodiment, the invention features a computer program product on a computer-readable medium for generating a library design for a combinatorial library of materials. The computer program includes instructions operable to cause a programmable processor to receive an input defining one or more sources and one or more destinations, receive an input defining a first mapping, use the first mapping to calculate a composition of one or materials assigned to one or more cells in the destination, and generate a data file defining the library design. Each source is electronic data representing a component to be used in preparing the combinatorial library. Each destination

is electronic data representing an arrangement of cells. The first mapping is electronic data defining a distribution pattern for assigning a component to cells in the arrangement. The distribution pattern includes a minimum and a maximum amount of the component to be assigned to any cell of the arrangement and a gradient to be applied between the minimum and maximum amounts of the component across the plurality of cells. The data file includes electronic data representing the sources, the destinations and the mapping.

**[0012]** Implementations of the invention can include one or more of the following advantageous features. The computer program includes instructions operable to cause a programmable processor to display a representation of the library design graphically describing the composition of one or more materials assigned to one or more of the cells. The data file includes electronic data representing one or more sets of properties, each set of properties being associated with one of the sources, the destinations or the mapping. The input defining the sources and destinations includes an input from a graphical input device.

**[0013]** The input defining a first mapping includes a selection from a set of available mapping types. The set of available mapping types includes a one to one mapping of a component from a source to a cell in the arrangement and a one to many mapping of a component from a source to a plurality of cells in the arrangement, a many to many mapping of a plurality of components from a plurality of sources to a plurality of cells in the arrangement, a many to one mapping of a plurality of components from a plurality of sources to a cell in the arrangement, or a set of one or more user-defined equations. The gradient is selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression. The set of properties associated with the mapping comprises a source name, a source geometry, a destination name, a destination geometry, a gradient type, and a set of gradient parameters defining the gradient. The computer program includes instructions operable to cause a programmable processor to receive an input defining a second mapping and use the first and second mappings to calculate a composition of one or more materials assigned to one or more of the cells. The second mapping is electronic data defining a second distribution pattern for distributing a second component to cells in the arrangement. The second distribution pattern includes electronic data identifying a fixed amount of the second component to be assigned to one or more cells in the arrangement. The second distribution pattern includes electronic data identifying a minimum and a maximum amount of the second component to be assigned to any of the cells of the arrangement and a second gradient to be applied between the minimum and maximum amounts of the second component across the cells. The computer program includes instructions operable to cause a programmable processor to generate a modified library design by receiving an input redefining a source, a destination or a mapping; recalculating the composition of one or more materials assigned to one or more of the cells; and generating a data file defining the modified library design. The computer program includes instructions operable to cause a programmable processor to receive an input defining one or more parameters and the data file includes comprises electronic data representing the one or more parameters. Each parameter is electronic data corresponding to a process parameter and defining a parameter value for one or more cells of the arrangement. The parameter value varies between a minimum and a maximum amount. The arrangement comprises two or more cells, ten or more cells, or about ninety-six or more cells.

**[0014]** In another embodiment, the invention features a computer program product including instructions operable to cause a programmable processor to receive an input defining one or more parameters, and generate a data file defining the library design. Each parameter is electronic data corresponding to a process parameter and defining a parameter value for one or more cells of the arrangement. The parameter value varies between a minimum and a maximum amount. The data file includes electronic data describing the source elements, the destination elements, the mappings and the parameters.

**[0015]** Implementations of the invention can include one or more of the following advantageous features. The parameter value is defined to vary over time, across two or more cells in the arrangement, or over time and across two or more cells in the arrangement. The parameter value varies according to a gradient selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression. The parameter value corresponds to a process parameter selected from the group consisting of temperature, pressure, time, flow rate and stirring speed.

**[0016]** In another embodiment the invention features a computer program product on a computer-readable medium for generating a library design for a combinatorial library of materials. The computer program includes instructions operable to cause a programmable processor to create a library design by defining a set of design elements, generate a data file including electronic data describing the design and use the data file to cause an automated material handling apparatus to assemble the combinatorial library on a substrate. The set of design elements includes one or more sources representing components to be used in preparing the combinatorial library, one or more destinations, and one or more elements selected from the group consisting of a mapping defining a scheme for assigning one or more amounts of a component to one or more cells of an arrangement and a parameter corresponding to a process parameter. Each destination includes an arrangement of one or more cells. The parameter defines a parameter value for one or more cells of the arrangement, the parameter value varying between a minimum and a maximum amount.

**[0017]** Advantages that can be seen in implementations of the invention include one or more of the following. The invention allows users to design combinatorial libraries conceptually, while automatically performing a large number

of detailed calculations required for the exact assignment of materials at each library member in a process that is preferably invisible to the user, although it may be shown if desired. The user can visualize a conceptual library design and identify potential errors before undertaking actual library synthesis. Separation of library design from library synthesis allows the user to lay out a library design conceptually, without regard for the physical limitations of a particular destination substrate or synthesis apparatus. The library design can flexibly define variation of chemical composition across library members by specifying multiple, interdependent material gradients or ratios defining the composition of each library member. The library design can also include variation of process parameters over time or across library members, which enables the user combinatorially to explore the effect of changing process conditions on material composition. The output of the design process is a recipe file that allows the automated synthesis of a library corresponding to the conceptual design. Maintaining databases of chemical information, library designs and composition data speeds up library design, avoids the repetition of old experiments, and assists in the overall planning and execution of experiments necessary to explore the preparation and properties of diverse materials.

**[0018]** The details of one or more embodiments of the invention are set forth in the accompanying drawings and the description below. Other features and advantages of the invention will become apparent from the description, the drawings, and the claims.

## BRIEF DESCRIPTION OF THE DRAWINGS

**[0019]** FIG. 1 is a block diagram illustrating a system for computer-implemented design of a combinatorial library of materials.

**[0020]** FIG. 2 is a flow diagram generally illustrating a method of designing a combinatorial library of materials.

**[0021]** FIG. 3 is a flow diagram illustrating a method of designing a combinatorial library of materials.

**[0022]** FIG. 4 is a ternary phase diagram describing the design of a conceptual triangular library of cells containing a mixture of three components in varying degrees.

**[0023]** FIG. 5A is a user interface window for use by a user designing a combinatorial library of materials.

**[0024]** FIG. 5B is an example of a window pane of the system user interface for defining one or more stock materials.

**[0025]** FIG. 5C is an example of a dialog of the system user interface for defining a destination object.

**[0026]** FIG. 6A is an illustrative library design window of the system user interface including a pane for graphically defining a library by mapping.

**[0027]** FIG. 6B is an example of a dialog for defining a gradient mapping object.

**[0028]** FIG. 6C is an example of a mapping dialog displaying a sequence of defined mappings defining a library.

**[0029]** FIG. 7A is an illustrative library design window including a pane for defining a library using equations.

**[0030]** FIGS. 7B and 7C are illustrative dialogs for defining an equation object.

**[0031]** FIG. 8A is an illustrative library design window depicting an equation design.

**[0032]** FIG. 8B is an example of a dialog displaying the calculation of composition for a cell in an equation design.

**[0033]** FIG. 8C is an illustrative library design window depicting the composition of a combinatorial library.

**[0034]** FIG. 8D is an example of a dialog depicting the composition of a library member.

**[0035]** FIG. 9A is an example of a dialog for defining a process parameter object.

**[0036]** FIG. 9B is an example of a pane displaying the properties of parameter objects.

**[0037]** FIG. 10 is an example of a library design window depicting a virtual ternary library design mapped to a rectangular plate.

**[0038]** Like reference numbers and designations in the various drawings indicate like elements.

## DETAILED DESCRIPTION

**[0039]** As shown in FIGS. 1 and 2, a system 100 includes a computer 110 equipped with input/output devices 120. A typical user of system 100 is a chemist. Through user interface 160, the user initializes system 100 and generates a library design for a combinatorial library of materials using design module 130 (step 200). As used in this specification, a combinatorial library is a collection of two or more members that contain some variance in chemical composition, chemical amount, reaction conditions, and/or processing conditions, where a member is a single position in a library containing one set of chemicals subject to one set of reaction or processing conditions.

**[0040]** Based on the library design, design module 130 creates a set of material handling instructions, which may take the form of a data file or "recipe file" (step 210), which may be provided to synthesis module 140 (step 220). Synthesis module 140 implements the instructions, by causing material handling apparatus 180 to synthesize a combinatorial library specified by the design, for example (step 230). Implementation of material handling instructions from recipe files to synthesize libraries of materials is described in more detail in co-pending U.S. Application Serial No. 09/305,830, filed on May 5, 1999, which is incorporated herein by reference in its entirety. Alternatively, design module 130 stores the set of material handling instructions in a file or relational database in memory 150 for later modification

by design module 130 or implementation by synthesis module 140.

**[0041]** Using design module 130, the user designs a library by defining a set of design elements corresponding to a design workspace, one or more mappings or distribution schemes for assigning materials to individual library members, and, optionally, one or more process parameters to be applied to one or more library members. FIG. 3 shows a method of using system 100 to design a combinatorial library of materials in more detail. Through user interface 160, the user defines a workspace by defining one or more sources (step 300) and one or more destinations (step 310). As used in this specification, a source is a chemical or mixture of chemicals that will be used as a component in creating a library, while a destination is a conceptual arrangement of cells representing a combinatorial library. In one embodiment, a destination may represent a physical substrate in or on which a library is created. In other embodiments, however, a destination is not constrained to represent an actual physical substrate, but can correspond to a conceptual library environment. Thus, as shown in FIG. 4 for example, a user may design a ternary library of three components A, B and C on a triangular destination in which each apex of triangle 400 corresponds to a composition of 100 percent of the corresponding component, while design module 130 translates the triangular conceptual design to a conventional rectangular grid corresponding to locations on a wafer or wells in a microtiter plate, as will be described in more detail below. The user defines each source and destination by entering identifying information, which may cause design module 130 to create a corresponding source or destination data object having associated properties defined by the user input, as will be described in more detail below. Alternatively, the user defines a source or destination by retrieving a pre-defined source or destination from memory 150.

**[0042]** The definition of sources and destinations is described in more detail with reference to FIGS. 5A-C. The user defines the necessary sources (meaning components to be used in designing and synthesizing a library, which may include materials located at one or more destination regions as will be described below) and destinations using design window 500, which includes outline pane 510, definition pane 530 and graphical pane 540. Outline pane 510 depicts a hierarchical view of the library design and its contents. At the top level, outline pane 510 displays a list of library design folders 511, each containing a library design. The next level lists sub-folders corresponding to the contents of each design, including, for example, sources folder 512, destinations folder 513, chemicals folder 514, equations folder 515 and parameters folder 516. At the third level, outline pane 510 displays icons depicting the individual design elements, including, for example, sources 517, destinations 518, chemicals 519. equations and parameters. When the user selects an icon corresponding to a desired element, user interface 160 displays information relevant to that element - for example, selection of a source 517 may result in display of a dialog identifying the names of the source's constituent chemicals, or other relevant properties. The hierarchical view in outline pane 510 also includes an icon 520 representing a recipe file corresponding to the library design.

**[0043]** The user defines a set of sources (such as stock solutions containing one or more chemicals dissolved in a solvent) to be used in creating the library, by, for example, selecting "Stock Materials" tab 525 (or a corresponding button on toolbar 560, a menu item in menus 570 or the like), which causes definition pane 530 to display a stock materials layer. Appropriate source materials (*i.e.*, components for use in library design) can include chemical elements, chemical compounds or chemical compositions, which may themselves include one or more elements or compounds. Source materials can be in a gaseous, liquid or solid phase.

**[0044]** For each source material, the user assigns a source name in field 531, and may enter information defining the source properties, including attributes of each constituent chemical such as type (or subtype), name (selected, for example, from a list of defined chemicals), molecular weight, equivalents, structure, density and concentration into corresponding fields 532-539. Values corresponding to source properties may be entered in any convenient units and are converted to common units for subsequent calculations by design module 130. To facilitate graphic display, each source may be assigned a distinct color. As sources are defined, they are depicted as source icons 517 in sources folder 512 in outline pane 510. Each source is also represented by an icon or shape 541 in graphical pane 540, which may be manipulated by the user -- for example, by using a mouse or other input device to move or drag the icon to any desired location in graphical pane 540 or to resize the icon as desired.

**[0045]** To define a chemical (a single material component within a synthetic design, for example a reagent that is synthesized or purchased for use in a source), the user makes an appropriate selection, such as by selecting "Chemicals" tab 545 in layered definition pane 530 causing that pane to toggle to a chemical definition layer 550, as shown in FIG. 5B. Alternatively, the user selects New Chemical button 561 on toolbar 560, an appropriate entry from drop-down menus 570, or other selection device. The user enters the chemical's name into Chemical Name field 552 and enters information defining the chemical's properties, such as molecular weight, equivalents, structure and density, into corresponding fields 553, 554, 555 and 556. Optionally, the user also assigns a chemical "Type" — a user-selected label describing a class of chemicals that may be used as a design parameter in creating the library — by entering a name into Type field 551. Each defined chemical type may include one or more subtypes. Alternatively, the user may retrieve the relevant data for a pre-defined chemical or chemicals from a database in memory 150 and transfer the data directly into the corresponding fields of the chemical definition layer.

**[0046]** To facilitate implementation of a library design, in one embodiment design module 130 outputs a stock solution

preparation worksheet that can be used for the manual or automated preparation of actual stock solutions to be used to synthesize the library. After the stock solutions are prepared, the user may enter actual values for mass, volume and concentrations of stock solution components, enabling design module 130 to recalculate its usage of stock materials based on the actual composition of available stock solutions.

**[0047]** The user defines one or more destinations by selecting an appropriate button or menu item, such as New Destination button 563 on toolbar 560, and entering a destination name and geometry information. Each destination includes one or more regions, each of which may be represented as a cell or group of cells in an arrangement (*e.g.*, an array) of one or more cells. A destination can include an arrangement of two or more cells, preferably four, ten, twenty, or even ninety-six or more cells. The cells or regions of a destination may, but need not, correspond to members of the combinatorial library and/or locations on a physical substrate (such as a microtiter plate, wafer or the like) on which the library will be created. However, while the destination may correspond to the geometry of the ultimate physical substrate, it may also represent the library on a more conceptual level, and may correspond to an abstract intermediate in the ultimate library design as will be described in more detail below. A destination can encompass one or more library designs; conversely, a library design can encompass any number of regions or cells of a destination, from a single cell to the total number of cells associated with the destination. In the described embodiment, destinations are depicted as square or rectangular arrays. However, destinations and the libraries they represent may be designed in any convenient shape, such as square, rectangle, circle, triangle or the like. Selection of a desired arrangement is a choice that can be manipulated by this invention. Strategies for designing combinatorial libraries are described in co-pending U.S. Application Serial No. 09/156,827, filed September 18, 1998, and U.S. Patent No. 5,776,359, both of which are incorporated herein by reference.

**[0048]** Thus, the user defines a destination by, for example, entering a number of rows and columns defining a bounding matrix of the destination into fields 581 and 582 of Destination Property dialog 580 shown in FIG. 5C. Each defined destination is represented as destination icons 517 in destinations folder 513 and as an appropriately-sized empty arrangement 542 of the appropriate shape in graphical pane 550, which may be manipulated by the user, such as by dragging to desired locations in graphical pane 550 or by resizing, as described for sources above.

**[0049]** Referring again to FIG. 3, the user designs the combinatorial library by assigning components (including chemicals) from sources to destination regions to define the composition of each library member (step 320). In one embodiment, described in detail with reference to FIGS. 6A-6C, the user directly defines one or more mappings that represent the assignment of one or more components to one or more destination cells. After defining the necessary sources and destination, represented as circles 601-603 and arrangement 607, respectively, in graphical pane 600, the user designs the library by using toolbar 610 to define a sequence of one or more mappings, each of which embodies a scheme or pattern for assigning an amount of a component or components from a source or sources to a destination region (*i.e.*, a cell or group of cells), or from a destination region to one or more other cells of the same or a different destination. As described below, mappings can be defined from a single source to a single destination region, from one source to multiple destination regions or from multiple sources (or destination regions) to multiple destination regions. The user may define a mapping by specifying that one or more components are to be assigned to one or more destination regions in uniform amounts or in varying amounts defined by a mathematical gradient or by a set of one or more governing equations applied to one or more destination regions, or by some combination of these methods.

**[0050]** To define a mapping, the user selects a mapping mode by, for example, selecting the appropriate button in toolbar 610. In one embodiment, to define a "one-to-one" mapping assigning a single component to a single destination cell the user selects one-to-one mapping button 615. The user then selects a desired source, for example by highlighting an icon or shape in graphical pane 600 such as circle 601. Next, the user selects a destination cell, for example by selecting a cell 620 in destination arrangement 607. The user is then prompted to enter an amount of the selected component to be assigned to the selected destination cell. Alternatively, the user may specify the amount of the component to be assigned to the destination cell by defining an equation as will be described below.

**[0051]** The user may define a mapping from multiple sources (including multiple regions in one destination) to multiple regions in another destination (or, if desired to another set of regions in the same destination) by, for example, selecting "many-to-many" mapping button 614. The user selects a group of cells in the starting destination, for example by dragging a cursor over the desired cells in destination arrangement 607, and a group of cells in the target destination (which may or may not be the same as the starting destination). The group of target cells may include any number of cells in the destination, and may include one or more rows or columns of cells, or parts of one or more rows or columns. Design module 130 prompts the user to input an amount of a component or components to be assigned from the selected starting cells to the selected target cells through user interface 160.

**[0052]** Optionally, the user may define a one-to-one or many-to-many mapping by reference to an appropriate text file, such as, for example, a tab-delimited spreadsheet file generated by Microsoft® Excel, by selecting an appropriate button 616 or 617. Design module 130 prompts the user to identify a source or sources and destination region or regions, and prompts the user to select a file containing the desired mapping information. Design module 130 assigns the selected component or components to the cells of the selected destination according to the contents of the selected

file. Thus, for example, the selected file may contain a tab-delimited array of constant values used to assign components to the corresponding cells of a selected destination array. Alternatively, design module 130 may calculate the amount of one or more components to be assigned to each cell in a selected destination based on equations, such as exponential, logarithmic, polynomial or geometric expressions or the like, contained in the selected file.

**[0053]** The user defines a mapping from a source to multiple destination cells by, for example, selecting a "one-to-many" mapping button 613. Design module 130 prompts the user to select a desired source and a group of cells in a desired destination, as described above. Design module 130 then prompts the user to specify a distribution scheme to be applied over the selected destination cells, for example defining a linear distribution gradient by entering starting and ending amounts, a direction and a distribution pattern (such as rectangular, triangular or other desired shape).

**[0054]** FIG. 6B shows one implementation of a dialog for defining a mapping distribution in more detail. Dialog 630 includes a pane 635 of radio buttons providing the user with a choice of various gradient shapes, such as rectangular or triangular. In pane 640, the user selects a gradient orientation — the direction or directions in the destination array along which the amount of the component increases. The user inputs the minimum and maximum values for the gradient in fields 645 and 650, and enters a number of rows or columns in the destination specifying the step size of the gradient in field 655. Design module 130 calculates an amount for each selected cell in the destination, beginning with the minimum amount in the first cell and increasing to the maximum amount according to the specified gradient.

**[0055]** In other embodiments, user interface 160 and design module 130 can be configured to define mappings based on other distribution schemes. For example, while the embodiment shown in FIG. 6B illustrates a dialog for defining a linear gradient, user interface 160 and design module 130 can be configured to define gradients according to one or more other well known mathematical forms, such as exponential, logarithmic, polynomial or geometric functions. Likewise, design module 130 can be configured to define "many-to-one" mappings for assigning amounts of material from multiple sources to a single destination region, using constant amounts of material from each source or varying amounts defined by gradients as described above. In still another embodiment, design module 130 can be configured to permit mapping from one source or sources to one or more others sources (or from a destination region or regions) to one or more sources.

**[0056]** While the embodiment shown in FIG. 6B provides for the definition of the gradient without reference to specific units of measure, user interface 160 and design module 130 can be configured to permit the user to input values in any convenient measure, such as, for example, units of molarity, weight, volume or thickness. In such embodiments, design module 130 automatically converts the selected units into appropriate units for calculation of mapping amounts, relieving the user of responsibility for making the necessary conversions. Thus, the user may define the sources for a library design using units that are most convenient for preparing stock solutions of components and design the library in another set of units more appropriate for that purpose, while design module 130 outputs a recipe file in still another set of units appropriate for synthesis of the library.

**[0057]** The user may view the properties of each defined mapping object (*e.g.*, sources, destinations, amounts, shape, and the like) and the overall mapping sequence through an appropriate mapping dialog, such as dialog 660 in FIG. 6C, accessed, for example, by selecting an appropriate menu item, toolbar button or other graphical device in user interface 160. The results of applying each defined mapping to a selected destination are displayed in graphical pane 600, which graphically depicts the composition of each destination region in the current library design. In the embodiment illustrated in FIG. 6A, composition data for destination arrangement 607 is displayed in layered chart form, with each cell in the destination being divided into colored or patterned layers or bars the size of which represents the relative amount of each component assigned to that cell. By selecting or unselecting the check box associated with each source (or chemical, depending on the selected view option) in outline pane 670 in FIG. 6A, the user may view the relative proportion of some or all components assigned to a given cell. Thus, for example, if the user deselects source A check box 675, design module 130 removes the layer corresponding to that source from each cell in array 607, allowing the user to view the relative proportions of the remaining components without regard to the amount of that source assigned to each destination region. Optionally, the user can view composition data in the form of an set of pie charts, described in more detail in connection with FIG. 8C, below, with each individual pie chart being divided into colored wedges depicting the relative amount of a corresponding component assigned to that destination region. The user can also access numerical compositional data in spreadsheet form by selecting an appropriate menu item, toolbar button or similar graphical device in user interface 160.

**[0058]** User interface 160 and design module 130 are also configured to enable the user to define a distribution scheme using systems of one or more equations defining the amount of a component or components, or the ratio between two or more such components, to be assigned to one or more destination regions. The user can employ such a "design by equations" mapping scheme to define mappings for the entire combinatorial library, or to define one or more mappings of a multi-mapping library design in combination with the gradient mapping implementation discussed above.

**[0059]** As shown in FIG. 7A, the user defines an equation by selecting an appropriate menu item or toolbar button, such as equation design button on toolbar 610, causing user interface 160 to display equation design arrangement

705 and associated equation design toolbar 710 in pane 700. The user initiates equation design by selecting Equation Design button 711, and partitions array 705 into regions, such as regions 706, 707, 708 and 709, for example by selecting the desired regions with a mouse or other input device. Selection of row partition or column partition buttons 715 and 716 causes design module 130 to insert a row or column header, such as column header 720, and creates a group of destination cells — for example, the group of cells in region 706 — that will be governed by any equations assigned to the corresponding header. By repeating the partitioning operation with various sizes of destination regions, the user can create multiple row and column headers capable of applying multiple equations to the cells of destination arrangement 705 as will be described below.

**[0060]** The user may assign a component (*i.e.*, a source or sources, including a chemical or chemicals) to a header by selecting the appropriate icon (*e.g.*, icon 731) from the current library design folder in outline pane 730, and dragging the selected source and dropping it into the desired header 720 in destination arrangement 705. This action causes design module 130 to assign the component represented by source icon 731 to all cells assigned to header 720 for use in equations governing those cells as described below. Optionally, the user may assign components (sources or chemicals) to one or more individual cells or groups of cells by dragging the selected component and dropping it into the desired cell or cells. The user may also assign multiple components to a destination by first defining an appropriate array of sources- for example an array of different chemicals of the same type — and dragging the source array onto the desired destination.

**[0061]** The user defines an equation by, for example, selecting a desired header and causing design module 130 to prompt the user to enter the relevant equation properties, for example through an equation property dialog 740 as shown in FIG. 7B. In dialog 740, the user defines a ratio equation describing a relationship between, for example, two or more components or chemical types as a sum of weighted terms. In fields 742, the user identifies the desired terms, which may include user-defined types or subtypes (*e.g.* catalysts, co-catalysts, solvents, initiators, monomers, surfactants, ligands, metals and the like), sources, chemicals or synthesis parameters such as total mass, total volume and the like. In one embodiment, terms in fields 742 may be selected from a list of available types, sources, chemicals and synthesis parameters by activating an arrow button 744 associated with a field 742 that invokes a pull-down menu identifying the available choices that have been defined as discussed above. The user enters coefficients defining the weighting of the selected term in coefficient fields 746. Additional types or subtypes, sources, chemicals or synthesis parameters can be incorporated in an equation by selecting box 748, which appends an additional line 750 to the equation, with additional term and coefficient fields 752 and 754. The user also selects an appropriate unit in unit field 755. Selection of OK button 756 causes design module 130 to assign the specified equation to the selected header. An icon representing the newly defined equation object is added to Equations folder 736 in outline pane 730.

**[0062]** Referring to FIG. 7C, more complex relationships can be defined by using coefficient functions, accessed in this embodiment by selecting coefficient box 760. This feature permits the user to use equations to define gradients to be applied across the cells in a region governed by a particular equation. As described above, the user selects appropriate terms (types, sources, chemicals, synthesis parameters) in term fields 762, and enters minimum and maximum coefficient values in fields 763 and 764, entering a step value for the gradient in step width field 765. The user then selects a desired function defining the change in coefficient values, such as linear, exponential or logarithmic functions, in function field 767, and selects a gradient direction, such as horizontal, vertical or diagonal, in direction field 768. A starting point for application of the gradient is selected using radio buttons 769. Selection of OK button 770 causes design module 130 to assign the defined function to the selected header, and to add an icon representing the equation object to the Equations folder in outline pane 730.

**[0063]** The user may assign equations to individual destination cells or groups of cells. A pre-defined equation can be assigned to a cell or group of cells, for example by selecting the equation icon from Equations folder 736 in outline pane 730 and dragging the equation to a desired cell or group of cells, or dragging the equation to a header governing a desired group of cells. The user may view a list of all equations defined for a particular cell, group of cells, or for the entire destination, for example in an equation list dialog window, and may copy equations from one cell or group of cells and assign those equations to another cell or group of cells, or to a header governing another group of cells.

**[0064]** FIG. 8A depicts a pane 800 illustrating a destination 810 for which a number of governing equations have been defined as described above. The user accesses this equation view of destination 800 by, for example, selecting an appropriate menu item or toolbar button, or by selecting arrangement 705 in FIG. 7A or array 607 in FIG. 6A with a mouse or other input device. Destination 810 includes rows and columns of cells 815 that correspond to the cells of arrangements 607 and/or 705. In this example, each cell 815 is depicted as including an equation designated as E7, E8, E9 or E10. The equations themselves are displayed as items in Equations folder 806 in outline pane 805.

**[0065]** Thus, for example, cells 801 to which equation E8 is assigned are subject to the equation

[Mole Equiv.] CoCatalyst = 1.0 * Catalyst,

where CoCatalyst and Catalyst are chemical Types defined in the Chemicals layer of the corresponding definition pane. Each cell 801 is also governed by equations appearing in headers located above the column and to the left of the row in which that cell appears. The cell identified by reference numeral 802, for example, is subject to the following equations:

[Mole Equiv.] CoCatalyst = 0.1 * Catalyst

[uL] TotalVolume = 200

[mg] Substrate = 0.12 * Total Mass

[Mole Equiv.] Catalyst = 0.0001 * Substrate

while the cell identified by reference numeral 803 is subject to the following equations:

[Mole Equiv.] CoCatalyst = 0.1 * Catalyst

[uL] TotalVolume = 200

[mg] Substrate = 0.12 * Total Mass

[Mole Equiv.] Catalyst = 0.01 * Substrate

As discussed above, the location of a given cell 801 also determines which specific components (chemicals or sources) are to be used to supply the Types specified by the relevant equations. Thus, for cell 802 discussed above, design module 130 will use Sources SolvA, SubB, CatD and CoCatE for Types Solvent, Substrate, Catalyst and CoCatalyst, respectively, in solving the set of equations that determine the composition of the corresponding region. That is, design module 130 will solve the following set of equations to calculate the composition of cell 802:

[Mole Equiv.] CoCatE = 0.1 * CatD

[uL] TotalVolume = 200

[mg] SubB = 0.12 * Total Mass

[Mole Equiv.] CatD = 0.0001 * SubB

**[0066]** The use of subtypes provides the user additional flexibility in designing a library using equations. For example, a user may design a library for copolymerizing pairs of monomers, with the monomers being added at different times during the polymerization reaction. By defining two chemical subtypes — for example, "first monomer" and "second monomer" — under single chemical type "monomer", the user may define the total amount of combined monomer using one equation (*e.g.*, [(mg) monomer = 0.2 Total Mass]), while defining the ration of the first monomer to the second monomer using a second equation (*e.g.*, [(mg) first monomer = 0.3 second monomer]).

**[0067]** In one embodiment, the user may cause design module 130 to verity that the set of defined equations is solvable at any time during the library design process, for example by selecting Check Mode button 812. In response to this selection, design module 130 performs a number of checks to determine whether the user has provided sufficient

information to enable design module 130 to solve the set of equations. Thus, for example, design module 130 determines whether the user has provided all source information, such as chemical molecular weight, concentration, density and the like, that will be required by the set of equations. If design module 130 determines that all necessary source information has not been defined, design module 130 prompts the user to enter the necessary information through user interface 160. Design module 130 also determines whether the number of defined equations matches the number of defined sources (and whether chemicals or sources of all appropriate Types have been assigned to each cell) and verifies that no equations are duplicated. For any cells that fail this equation check, design module 130 informs the user of an equation error through user interface 160, for example by displaying an appropriate error message or displaying the destination array with failed cells identified by an appropriate color or pattern, such as by displaying cells for which sufficient information has been defined in green and all other cells in red. Optionally, design module 130 also informs the user of the reason or reasons why the equations defined for a given cell cannot be solved.

**[0068]** Upon receiving user input indicating that equation design is complete (for example, by selection of Solve Equations button 813), design module 130 uses conventional matrix algebra techniques to solve the equations defined for a given destination to calculate the composition of the corresponding destination cells. substituting the appropriate Chemicals and Sources for Types included in the set of equations defined for each cell. Thus, for example, design module 130 uses techniques such as LU decomposition to solve a set of defined ratio equations, providing results in the form $X = X_1 + X_2$, where $X_1$ is a sub-vector of chemical masses and $X_2$ is a subvector of volumes of stock materials. Design module 130 may be configured to accept and solve other types of equations, such as mass equations defined as:

$$[-I]X_1+[D]X_2 = 0$$

or,

$$\left[-I\ D\right]\begin{bmatrix}X_1\\X_2\end{bmatrix}=0,$$

where $X_1$ is a sub-vector of chemical masses and $X_2$ is a sub-vector of volumes of stock materials, I is the identity matrix and D is the density matrix.

**[0069]** The calculations with which design module 130 solves the set of equations for each cell may be internal to the computer and invisible to the user; optionally, design module 130 displays the calculations in a window through user interface 160. As described above in connection with Check Mode button 812, when solving equations design module 130 optionally identifies each cell for which the assigned equations have a valid solution with an appropriate color, pattern or other visual display scheme, while identifying cells for which the assigned equations are not solvable with another appropriate display scheme (such as, for example, displaying cells with a valid solution in green and other cells in red). Design module 130 is configured to allow the user to "diagnose" the reason for the failure to solve a cell's equations by, for example, displaying in response to appropriate user input an Equation Matrix dialog 830, as shown in FIG. 8B. For a selected cell, here cell 802 in array 810, dialog 830 displays a status for the cell (*e.g.*, "Equation solving failed"), as well as a spreadsheet 835 with regions corresponding to values derived from the equations assigned to the selected cell (840), values calculated from stock material concentrations defined in the definition pane (845) and equation solutions for chemical mass and stock solution volume (850). In the example depicted in FIG. 8B, solutions region 850 reveals that the calculated volume for SolvA is negative, rendering the equations assigned to cell 802 not solvable.

**[0070]** As shown in FIG. 8C, the user may view a graphic display of the calculated composition data resulting for an equation design by selecting an appropriate menu item of toolbar button, such as Display Data button 856 of graphical pane 855. The user may elect to view composition data by chemical mole or mass ratio, for example by selecting chemical button 860 and mole or mass buttons 862 or 863, respectively; alternatively, composition data may be displayed by source volume ratio by selecting source button 865 and corresponding volume button 866. Selection of pie chart button 868 causes design module 130 to display the composition data as an arrangement 870 of cells 872. Each cell 872 contains a pie chart 875 representing the calculated composition of the corresponding destination region determined by solution of the set of equations assigned to that cell. The relative proportion of each component assigned to the destination region (in units determined by the selected viewing option — volume for stock material solutions, mass or molarity for chemicals) is represented in each chart 875 by the size of a corresponding pie wedge depicted in a color or pattern associated with a given component (*e.g.*, by colors assigned to each source component in Sources folder 877 in outline pane 880. By selecting or unselecting the check box associated with each source (or chemical, depending on the selected view option) in outline pane 880, the user may view the relative proportion of some or all

components assigned to a given cell. Thus, for example, if the user deselects SolvA check box 882, design module 130 removes the pie wedge corresponding to that source from each pie chart 875 in arrangement 870, allowing the user to view the relative proportions of the remaining components without regard to the amount of solvent (SolvA) assigned to each destination region. The user may also view the calculated composition data in layered chart form as described above in connection with FIG. 6A, above. Numerical composition data for each destination region may be displayed through a cell composition data dialog 885, as shown in FIG. 8D.

**[0071]** Referring again to FIG. 3, in one embodiment, design module 130 is configured to enable the user to incorporate varying process parameters into a library design through parameters specifying a scheme of varying values across one or more destinations. Parameters can include any external conditions, such as temperature, pressure, mixing speed, quench time, flow rate and the like. The user defines a parameter by, for example, selecting an appropriate menu item or toolbar button (step 330). Design module 130 prompts the user to enter the necessary information by displaying an appropriate dialog, such as Parameter Property dialog 900 shown in FIG. 9A. The user assigns a parameter name in name field 905 and selects a parameter type and appropriate units in fields 910 and 915. The user identifies one or more destinations in field 920 to which design module 130 will apply the defined parameter. In field 925, the user selects a scheme for varying the parameter values, which may include schemes such as temporal variation, spatial variation and the like, as well as combinations of such variation schemes. Design module 130 is configured to vary parameter values spatially, across one or more rows or columns, specified by the user in fields 930 and 935, respectively. Similarly, the user defines a temporal variation by specifying a time function (such as a linear function or a step function), a number of time steps and an appropriate time unit (such as seconds, minutes or hours) in fields 950, 940 and 945, respectively. The user may enter comments describing the parameter in comment field 955. Upon completion, signified, for example, by the user's selection of OK button 960, design module 130 stores the parameter in memory 180, adds a corresponding parameter icon to parameter folder 515 in outline pane 510, and allocates space in the parameter layer of definition pane 530, as will be described next.

**[0072]** As shown in FIG. 9B, a parameter layer 965 is accessed by selecting parameter tab 970 in definition pane 968. Parameter layer 965 includes an entry for each defined parameter, such as Temperature parameter 975 and Pressure parameter 980. Each defined parameter is identified by an expandable entry identifying the parameter type (975, 980), which, upon expansion, displays the parameter properties input through Parameter Property dialog 900, as discussed above, such as a name 976, a step identifier 977, a start time 978 for each step, and a description or value for the parameter at that step 979. As appropriate, parameter layer 965 includes a spreadsheet-type display 985 depicting a parameter value for each cell in the destination to which the parameter is assigned in field 920 of Parameter Property dialog 900, as described above. Design module 130 is configured to allow the user to enter parameter values manually into parameter layer 965; alternatively, design module 130 populates parameter values according to a variation scheme defined in Parameter Property dialog 900, such as applying a constant or gradient function to a selected group of destination cells. The user can modify parameter values through Parameter Property dialog 900, or directly through parameter layer 965.

**[0073]** When library design is complete, the user may optionally store design files, including some or all of the design information -- *ie.* the sources, destinations and parameters, as well as the mapping scheme and other related information — in memory 180. In one embodiment, design module 130 outputs a text file (or a tab-delimited spreadsheet file in a format suitable for a program such as Microsoft® Excel), describing the relative or absolute amounts of components to be deposited at each library member to allow a chemist to manually prepare the designed library. Alternatively, design module 130 can be configured to output an image file, such as Microsoft® PowerPoint file, depicting the graphical layer chart or pie chart display of composition data for a selected destination.

**[0074]** Design module 130 is also configured to generate a recipe file containing a set of synthesis instructions in a generic format that can be retrieved by synthesis module 140 for automated processing by material handling apparatus 180 (step 340 in FIG. 3). Appropriate apparatus 180 can include, for example, automated liquid handling robots, such as the RSP 900 Robotic Sample Processor, available from Cavro Scientific Instruments, Inc. of Sunnyvale, California. Apparatus 180 can also include automated systems performing different types of physical or chemical vapor deposition. In liquid handling, mixtures of solutions are typically dispensed in an array of miniature wells to create a library. In vacuum deposition, solid elements or chemicals or mixtures of solid elements or chemicals are vaporized and deposited as individual components on a substrate. The deposition may be controlled by a series of shutters and masks to manufacture the library. For an example of deposition equipment, see WO98/47613 (U.S. Application Serial No. 08/841,423), filed on April 22, 1997.

**[0075]** In one embodiment, an appropriate data file or recipe file includes an entry for each source, each destination, each parameter, and each mapping created as described above, such as shown in Table 1 for the component labeled "CatA" in the equation design illustrated in FIG. 8A.

Table 1

```
[COMPONENT_1]
compLabel= CatA
libRegBegin= NULL
libRegEnd= NULL
arrayGeom= RECT
numRows= 1
numColumns= 1

[MAPPING_1]
Source= CatA
SourceRect= (1,1),(1,1)
Destination= Plate
DestRect= (2,2),(7,11)
GradientType= LIN
GradientParams= 10.000000 0.0 0.0 -2.000000 0.000000 0.0 0.0 1 0
Tag=
```

Design module 130 graphically represents the recipe file for the current design as an icon 520 in outline pane 510 shown in FIG. 5A.

**[0076]** As described above, design module 130 creates a library design unconstrained by the physical limitations of available synthesis apparatus and library substrates. Thus, while the user may design a library using a destination arrangement containing the number of library members (*i.e.* individual reactors) in the same geometry (*e.g.*, the number of rows and columns) as the physical substrate on which the library will ultimately be prepared, design module 130 enables the user to design libraries without regard to these constraints. Thus, the user may design a conceptual "virtual" library containing vast numbers of individual members (thus spanning multiple physical libraries), yet connected by a central chemical concept. Similarly, the user may also design a library in a preferred design environment (*e.g.*, a geometry that best defines a library concept such as the ternary design shown in FIG. 4), while the design can be implemented in a different physical geometry for convenience of library synthesis. One such virtual library design is shown in FIG. 10. The user designs a library of varying compositions of sources A and B in ternary form on "Virtual Plate" destination 1000, with the amount of source A assigned to each cell determined by a linear gradient defined in equation 1010. Design module 130 then maps the 91 occupied cells of destination 1000 onto rectangular "Physical Plate" 1020 for implementation by conventional synthesis apparatus.

**[0077]** The user can also define a library design for use as a template in the design and preparation of multiple related libraries. Thus, for example, a library design of 96 different catalyst formulations may be used as a template to explore the polymerization of various organic monomers. Alternatively, a design can be defined for a portion of a single destination and used as a template to define multiple designs covering the entire destination — for example, the user may create a template design for a library of polymerization catalysts that covers only a single quadrant of an 8x12 destination and use the template to define a set of four library designs in which four different monomers are polymerized in the presence of the catalyst library. In this embodiment, the user designs the library as described above, with one source defined to correspond to one desired monomer, and stores the design in memory 150. The user may then retrieve the design and use design module 130 to create a series of library, one for each desired monomer, by simply replacing the defined monomer in the template design, recalculating the composition of each destination cell and generating the corresponding recipe file. More generally, the user may create a template design using a set of n design elements, where, for example, n defines the number sources used in the design, and instruct design module 130 and synthesis module 140 to generate a series of m libraries, where m>n and m is a number of actual sources used in preparing the libraries. Thus, while the library design may specify a combination of a limited number of design elements — for example, a quaternary library of inorganic materials in which each cell contains a mixture of four materials -- the library design can be implemented for a larger number of elements, by creating a set of libraries encompassing all possible combinations/iterations of sources from the set of available sources — for example, by creating all possible combinations of four materials from a set of six available materials. Similar template designs can be created for designs involving any design elements — for example, multiple equation coefficients, multiple parameter values, or any combination of elements.

**[0078]** In one embodiment, design module 130 is configured to interact with a database 150 associated with system 100 that is capable of archiving information pertaining to available chemicals, stock materials, composition data for

existing library designs and the like. In this embodiment, the user may search the database for chemicals based on relevant identifying information, such as chemical name, formula, identification number (*e.g.*, CAS number) or the like. The user may select any chemicals identified in such a search, and design module 130 downloads chemical attribute information into the Chemicals layer in the current library design (*e.g.*, definition pane 530 in FIG. SA). To facilitate archiving and tracking of existing library designs, the user may register one or more libraries on a designed destination in a database 150 associated with system 100. Design module 130 assigns each library so registered an identification number with which each library may later be retrieved from database 150. Similarly, the user may load composition data for one or more libraries on a destination to database 150 for later retrieval.

**[0079]** The design methods and programs of the present invention can be advantageously applied in connection with the design and synthesis of libraries or arrays of diverse materials. Preferably, such diverse materials are candidate materials (*e.g.*, catalysts) being evaluated for a desired chemical property, for example a capability to enhance a chemical process (*e.g.*, chemical reaction) of interest.

**[0080]** A library of such materials can be a physical array of candidate materials, comprising a substrate and two or more different candidate materials, and preferably four or more different candidate materials at separate portions of the substrate, corresponding to library members. Each candidate material can consist essentially of two components (or source materials -- *e.g.*, a combination of sources A and B). Alternatively, additional components can be incorporated in the library design, resulting in libraries of diverse materials having compositions that are essentially ternary, quaternary or higher order. Such higher-order compositions can be designed to include the same components (*e.g.*, A, B and C) in each composition, but in varying amounts or ratios, or alternatively, to include different components (*e.g.*, A, B and C; A, B and D; A, B and E; A, B and F, etc.) in two or more of the compositions. In one preferred library, the is a spatially addressable array of materials that comprises a substrate having a surface and nine or more materials having different compositions at nine or more discrete regions of the substrate surface, with each material-containing region consisting essentially of one material. The nine or more materials preferably comprising two or more common components of interest, A and B, with the amount of at least one of the common components, A, preferably varying incrementally and uniformly between the nine or more materials, such that the nine or more materials form a uniform compositional gradient with respect to component A. The gradient can be linear, exponential, *etc.,* as described above. The amount of one or more additional components (*e.g.*, component B) can also vary. Non-gradient applications are also considered, as explained above in connection with the various mappings. In a particularly preferred library, the array comprises eleven or more materials at eleven or more discrete regions of the substrate, and at least one of the materials comprises component A and an essential absence of component B.

**[0081]** Appropriate candidate materials can include elements, compounds or compositions comprising a plurality of elements and/or compounds, and can be in a gaseous, liquid or solid phase. Solid-phase materials are preferred for some applications. The particular elements, compounds or compositions to be included in a library of candidate materials will depend upon the particulars of the chemical phenomenon or process being investigated. However, the nature of the particular chemical phenomenon or process being investigated is not critical, such processes can include, for example, chemical reactions and chemical separations, among others.

**[0082]** For example, candidate materials can include compositions that catalyze reactions including activation of, breaking and/or formation of H-Si, H-H, H-N, H-O, H-P, H-S, C-H, C-C, C=C, C≡C, C-halogen, C-N, C-O, C-S, C-P, C-B and C-Si bonds among others. Exemplary chemical reactions for which reaction-enhancing materials may be identified according to the present invention include, without limitation, oxidation, reduction, hydrogenation, dehydrogenation (including transfer hydrogenation), hydration, dehydration, hydrosilylation, hydrocyanation, hydroformylation (including reductive hydroformylation), carbonylation, hydrocarbonylation, amidocarbonylation, hydrocarboxylation, hydroesterification, hydroamination, hetero-cross-coupling reaction, isomerization (including carbon-carbon double bond isomerization), dimerization, trimerization, polymerization, co-oligomerization (e.g. CO/alkene, CO/alkyne), co-polymerization (e.g. CO/alkene, CO/alkyne), insertion reaction, aziridation, metathesis (including olefin metathesis), carbon-hydrogen activation, cross coupling, Friedel-Crafts acylation and alkylation, Diels-Alder reactions, C-C coupling, Heck reactions, arylations, Fries rearrangement, vinylation, acetoxylation, aldol-type condensations, aminations, reductive aminations, epoxidations, hydrodechlorinations, hydrodesulfurations and Fischer-Tropsch reactions, asymmetric versions of any of the aforementioned reactions, and combinations of any of the aforementioned reactions in a complex reaction sequence of consecutive reactions. For chemical reactions, candidate materials can be generally classified as those materials which are chemically altered or consumed during the course of the reaction (e.g., co-reactant materials, cataloreactants) and those materials which are not chemically altered or consumed during the course of the reaction (e.g., catalysts, selective blocking moieties). In preferred applications, candidate materials are catalysts, which term, as used herein, is intended to include a material that enhances the reaction rate of a chemical reaction of interest or that allows a chemical reaction of interest to proceed where such reaction would not substantially proceed in the absence of the catalyst.

**[0083]** Appropriate candidate materials preferably include elements or compounds selected from the group consisting of inorganic materials, metal-ligand complexes and non-biological organic materials. In some applications, candi-

date materials will consist essentially of inorganic materials, consist essentially of metal-ligand materials, or consist essentially of non-biological organic materials. Moreover, in some applications, source and/or candidate materials will be compositions comprising mixtures of inorganic materials, metal-ligand materials, and/or non-biological organic materials in the various possible combinations.

**[0084]** Inorganic materials include elements (including carbon in its atomic or molecular forms), compounds that do not include covalent carbon-carbon bonds (but which could include carbon covalently bonded to other elements, e.g., $CO_2$), and compositions including elements and/or such compounds. Inorganic candidate materials that could be investigated in libraries designed according to the approaches described herein include, for example: noble metals such as Au, Ag, Pt, Ru, Rh, Pd, Ag, Os and Ir; transition metals such as Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Y, Zr, Nb, Mo, Ta, W and Re; rare-earth metals such as La, Ce, Pr, Nd, Sm, Eu, Tb, Th and U; alloys of noble metals, transition metals and/or rare-earth metals; metal oxides such as CuO, NiO and Co304; noble-metal-doped metal oxides such as noble-metal-doped CuO, NiO and Co304; multi-metal oxides such as binary oxides of Cu-Cr, Cu-Mn, Cr-Mn, Ni-Cr, Ni-Mn, Ni-Cu, Ni-Mo, Cu-Mo, Ni-Co, Co-Mo, Ni-Fe, Fe-Mo, Cu-Fe, Mn-Ag, Mn-Sn, Ag-Sn, Cu-Ag, Cu-V, Ag-V, Cu-V, Ni-V, Bi-Mo, Bi-V, Mo-V, V-Zr, V-Ti, Zr-Ti, V-Nb, Nb-Mo, V-P, P-Mo, Ni-P, P-Cu, Co-P, Co-Fe, P-Fe, Mg-V, Mg-Sn, V-Sn, K-Ti, K-Bi, Ti-Bi, Cr-Sb, Cr-V, Sb-V, Bi-Mo, Bi-Nb, K-Cr, K-Al, Al-Cr, Zn-Cu, Zn-Al, Cu-Al, La-Cr, La-Zr, Cr-Zr, La-Mo, Mo-Zr, La-W, W-Zr, Mo-W, W-V, Cu-W, Bi-W, Fe-Sb, Fe-V and Ni-Ta, Ni-Nb and Ta-Nb, and such as ternary oxides of Cu-Cr-Mn, Ni-Cr-Mn, Ni-Cu-Mo, Ni-Co-Mo, Ni-Fe-Mo, Cu-Fe-Mo, Mn-Ag-Sn, Cu-Ag-V, Cu-Ni-V, Bi-Mo-V, V-Zr-Ti, V-Nb-Mo, V-P-Mo, Ni-P-Cu, Co-P-Fe, Mg-V-Sn, K-Ti-Bi, Cr-Sb-V, Bi-Mo-Nb, K-Cr-Al, Zn-Cu-Al, La-Cr-Zr, La-Mo-Zr, La-W-Zr, Mo-W-V, Cu-Mo-W, Bi-Mo-W, Bi-V-W, Fe-Sb-V and Ni-Ta-Nb; metal carbides such as PdC; metal sulfates, metal sulfides, metal chlorides, metal acetates, polyoxometallates (POM); metal phosphates such as vanadylpyrophosphates (VPO); Bronstead acids such as HF; Lewis Acids such as AlCl3; and mixtures of any of the aforementioned inorganic materials, among others. Exemplary inorganic material libraries could include, for example, triangular-shaped arrays of ternary metal oxides (e.g. such as oxides of the ternary metal partners described above) with single metal oxide compounds at each corners, binary metal oxide compositions along each of the sides with varying ratios of constituents, and ternary metal oxide compositions in the interior regions of the triangular array with varying ratios of constituents. Libraries of inorganic candidate materials can be prepared, for example, according to the methods disclosed in U.S. Patent No. 5,776,359 to Schultz et al.

**[0085]** Metal-ligand complexes comprise a central metal atom or ion surrounded by, associated with and/or bonded to other atoms, ions, molecules or compounds — collectively referred to as "ligands" — typically through a carbon (to form, e.g., an organometallic), nitrogen, phosphorous, sulfur or oxygen atom and/or one or more linker moieties. The one or more ligands typically bind to one or more metal center and/or remain associated therewith, and by such association, modify the shape, electronic and/or chemical properties of the active metal center(s) of the metal-ligand complex. The ligands can be organic (*e.g.*, ç$^1$-aryl, alkenyl, alkynyl, cyclopentadienyl, CO, alkylidene, carbene) or inorganic (*e.g.*, $Br^-$, $Cl^-$, $OH^-$, $NO^{2-}$, *etc.*), and can be charged or neutral. The ligand can be an ancilliary ligand, which remains associated with the metal center(s) as an integral constituent of the catalyst or compound, or can be a leaving group ligand, which may be replaced with an ancillary ligand or an activator component. Exemplary metals / metal ions include ions derived from, for example, simple salts (*e.g.*, $AlCl_3$, $NiCl_2$, *etc.*), complex or mixed salts comprising both organic and inorganic ligands (*e.g.*, $[(\eta 5\text{-}C_5Me_5)IrCl_2]_2$, *etc.*) and metal complexes (*e.g.*, $Gd(NTA)_2$, CuEDTA, *etc.*), and can generally include, for example, main group metal ions, transition metal ions, lanthanide ions, *etc.*

**[0086]** Libraries of metal-ligand candidate materials designed according to the methods and programs described herein can be prepared, for example, according to the methods disclosed in PCT Patent Application WO 98/03521 of Weinberg et al. Briefly, a desired ligand can be combined with a metal atom, ion, compound or other metal precursor compound. In many applications, the ligands will be combined with such a metal compound or precursor and the product of such combination is not determined, if a product forms. For example, the ligand may be added to a reaction vessel at the same time as the metal or metal precursor compound along with the reactants. The metal precursor compounds may be characterized by the general formula $M(L)_n$ (also referred to as $ML_n$ or $M\text{-}L_n$) where M is a metal and can include metals selected from the group consisting of Groups 5, 6, 7, 8, 9 and 10 of the Periodic Table of Elements. In some embodiments, M can be selected from the group consisting of Ni, Pd, Fe, Pt, Ru, Rh, Co and Ir. L is a ligand and can be selected from the group consisting of halide, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, heterocycloalkyl, substituted heterocycloalkyl, aryl, substituted aryl, heteroaryl, substituted heteroaryl, alkoxy, aryloxy, hydroxy, boryl, silyl, hydrido, thio, seleno, phosphino, amino, and combinations thereof, among others. When L is a charged ligand, L can be selected from the group consisting of hydrogen, halogens, alkyl, substituted alkyl, cycloalkyl, substituted cycloalkyl, heteroalkyl, heterocycloalkyl, substituted heterocycloalkyl, aryl, substituted aryl, heteroaryl, substituted heteroaryl, alkoxy, aryloxy, silyl, boryl, phosphino, amino, thio, seleno, and combinations thereof . When L is a neutral ligand, L can be selected from the group consisting of carbon monoxide, isocyanide, nitrous oxide, $PA_3$, $NA_3$, $OA_2$, $SA_2$, $SeA_2$, and combinations thereof, wherein each A is independently selected from a group consisting of alkyl, substituted alkyl, heteroalkyl, cycloalkyl, substituted cycloalkyl, heterocycloalkyl, substituted heterocycloalkyl, aryl, substituted aryl, heteroaryl, substituted heteroaryl, alkoxy, aryloxy, silyl, and amino. Specific

examples of suitable metal precursor compounds include $Pd(dba)_2$ (dba = dibenzylydieneacteone), $Pd_2(dba)_3$, $Pd(OAc)_2$ (Ac = acetate), $PdCl_2$, $Pd(TFA)_2$, (TFA = trifluoroacetate), $(CH_3CN)_2PdCl_2$, and the like. In this context, the ligand to metal precursor compound ratio is in the range of about 0.01:1 to about 100:1, more preferably in the range of about 0.5:1 to about 20:1. The metal atom, ion or metal precursor may be supported or not. Supports may be organic or inorganic. Similar to the ligands, the support may be an L. In other embodiments, the support will not form part of the metal precursor and suitable supports include silicas, aluminas, zeolites, polyethyleneglycols, polystyrenes, polyesters, polyamides, peptides and the like. Specific examples of Pd supported metals include Pd/C, $Pd/SiO_2$, $Pd/CaCO_3$, $Pd/BaCO_3$, Pd/aluminate, Pd/aluminum oxide, Pd/polystyrene, although any of the metals listed above could replace Pd in this list, e.g., Ni/C, etc. In other applications, the ligand will be mixed with a suitable metal precursor compound prior to or simultaneous with allowing the mixture to be contacted to the reactants. When the ligand is mixed with the metal precursor compound, a metal-ligand complex may be formed, which may be employed as a candidate material.

**[0087]** Non-biological organic materials include organic materials other than biological materials. Organic materials are considered to include compounds having covalent carbon-carbon bonds. Biological materials are considered to include nucleic acid polymers (e.g., DNA, RNA) amino acid polymers (e.g., enzymes) and small organic compounds (e.g., steroids, hormones) where the small organic compounds have biological activity, especially biological activity for humans or commercially significant animals such as pets and livestock, and where the small organic compounds are used primarily for therapeutic or diagnostic purposes. While biological materials are of immense commercial interest with respect to pharmaceutical and biotechnological applications, a large number of commercially significant applications involve chemical processes that are enhanced by other than biological materials. Moreover, while fundamental screening approaches for many pharmaceutical and biological activities are known or readily adapted from known approaches, screening approaches for non-biological materials have not heretofore been widely investigated and reported. Although candidate materials being screened are preferably not, themselves, biological organic materials, candidate materials included in libraries designed according to the invention (e.g., inorganic materials) can be employed to enhance reactions directed to producing a biological organic material as the product of a chemical reaction (e.g., materials that enhance chemical-based, non-enyzmatic DNA synthesis, or materials that enhance a synthetic, non-enyzmatic route to a particular hormone or steroid).

**[0088]** The amount of an individual candidate material located in a particular library member varies depending upon the required application and the method by which the library is prepared. For thin films, for example, the amount of material will depend on the surface area of the film and the required thickness of the film, each of which will, in turn, vary depending upon the chemical process of interest. For catalyst applications, the geometry of the reactor, and the required residence time or contact time of reactants in the reactor, among other factors, will also be important. In general, the amount of an individual candidate material is typically not more than about 25 mg, preferably not more than about 10 mg, and can be not more than about 7 mg, not more than about 5 mg, not more than about 3 mg and not more than about 1 mg. In preferred embodiments, the amount of an individual candidate material can range from about 0.1 ìg to about 100 mg, preferably from about 1 ìg to about 10 mg, more preferably from about 10 ig to about 10 mg and most preferably from about 100 ìg to about 1 mg.

**[0089]** Libraries designed according to the methods discussed above can be prepared on any convenient substrate, including any suitable material having a rigid or semirigid surface on which the candidate materials can be formed or deposited or to which the candidate materials can be linked. The substrate preferably consists essentially of materials that are inert with respect to the materials and chemical processes of interest. Certain materials will, therefore, be less desirably employed as a substrate material for certain reaction process conditions (e.g., high temperatures — especially temperatures greater than about 100 °C — or high pressures) and/or for certain reaction mechanisms. The substrate material is also preferably selected for suitability in connection with microfabrication techniques, such as selective etching (e.g., chemical etching in a liquid or gaseous phase, plasma-assisted etching, and other etching techniques) photolithography, and other techniques known or later-developed in the art. Silicon, including polycrystalline silicon, single-crystal silicon, sputtered silicon, and silica ($SiO_2$) in any of its forms (quartz, glass, etc.) are preferred substrate materials. Other known materials (e.g., silicon nitride, silicon carbide, metal oxides (*e.g.*, alumina), mixed metal oxides, metal halides (*e.g.*, magnesium chloride), minerals, zeolites, and ceramics) may also be suitable for a substrate material. Organic and inorganic polymers may also be suitably employed in some applications of the invention.

**[0090]** Appropriate substrates may, but need not necessarily, have at least one substantially flat, substantially planar surface, and may preferably, but not necessarily, be a substantially planar substrate such as a wafer. The surface of the substrate can be divided into physically separate regions and can have, for example, dimples, wells, raised regions, etched trenches, or the like formed in the surface. In still other embodiments, small beads or pellets may be the substrate, and such beads or pellets may be included in an array, for example, for example, placing the beads within dimples, wells or within or upon other regions of the substrate's surface. Frits can be used to hold such beads or pellets in place. In other applications, the substrate can be a porous material. The substrate can, and is preferably, passive — having an essential absence of any active microcomponents such as valves, pumps, active heating elements, active

mixing elements. The substrate also preferably has an essential absence of passive microcomponents such as microfluidic channels or apertures used for fluid distribution, heat-transfer elements, mass-transfer elements (e.g., membranes), etc., or combinations thereof. In some applications, however, the substrate can include such active microcomponents or such passive microcomponents. In a preferred application, the substrate has a substantially flat upper surface with a plurality of substantially coplanar indentations or wells of sufficient depth to allow a quantity of candidate material to be deposited, formed or contained therein. The overall size and/or shape of the substrate is not limiting to the invention. The size can be chosen, however, to be compatible with commercial availability, existing fabrication techniques (e.g., silicon wafer availability and/or fabrication), and/or analytical measurement techniques. Generally, the substrate will be sized to be portable by humans and/or to be manipulated by automated substrate-handling devices. Hence, two inch and three inch wafers are suitably employed. The choice of an appropriate substrate material and/or form for certain applications will be apparent to those of skill in the art based on the guidance provided herein.

**[0091]** In libraries prepared from library designs generated according to the methods discussed above, the candidate materials are generally deposited in a plurality of library members arranged on a substrate. The desired configuration of the candidate material with respect to the substrate depends upon the application. Thus, for example, for a library of candidate catalyst materials, the library can be configured in any design that allows for one or more reactants to contact the candidate material during the chemical reaction or other chemical process. Hence, it can be appreciated that the exact configuration of the candidate materials and the substrate are not limiting to the invention. Typical configurations generally allow for fluid flow past and around a candidate material formed on a surface of a reaction cavity, for unidirectional flow of reactants through a porous substrate or through a bed of beads, or for flow of reactants into and out of a well comprising a porous or non-porous substrate.

**[0092]** The candidate materials are preferably spatially separated in the library of candidate materials, preferably at an exposed surface of the substrate, such that the array of materials can, for example, be integrated with a plurality of microreactors to include different candidate materials within different microreactors for screening individual candidate materials for chemical properties of interest. Moreover, individual library members are also preferably separately addressable, for example, for analytical characterization thereof. The two or more different candidate materials are therefore preferably located at discrete, non-contiguous, individually addressable regions of the substrate, with the regions being spaced to accommodate inclusion into a plurality of microreactors. The different candidate materials may, nonetheless, also be contiguous with each other (e.g. as in a continuous gradient of different material compositions). However, even where a spatially separated, individually addressable array of candidate materials is desired in the ultimate physical library, the library design need not have these features, which may be incorporated by appropriate synthesis apparatus or by software controlling such apparatus.

**[0093]** If the two or more candidate materials are to be deposited on distinct, individually addressable regions of the substrate, the separation between adjacent regions can range from about to about 50 im to about 1 cm, more preferably from about 100 im to about 7 mm, and most preferably from about 1 mm to about 5 mm. The inter-region spacings can be not more than about 1 cm, not more than about 7 mm, not more than about 5 mm, not more than about 4 mm, not more than about 2 mm, not more 1 mm, not more than about 100 im, and not more than about 50 ìm. Exemplary inter-regions spacings (center-to-center) based on preferred embodiments of the invention are 4 mm for having 256 addressable regions on a three-inch wafer substrate, and 2 mm for having 1024 addressable regions on a three-inch wafer substrate. As such, the surface density of discrete candidate material regions can range from about 1 region/$cm^2$ to about 200 regions/$cm^2$, more preferably from about 5 regions/$cm^2$ to about 100 regions/$cm^2$, and most preferably from about 10 regions/$cm^2$ to about 50 regions/$cm^2$. The planar density can be at least 1 region/$cm^2$, at least 5 regions/$cm^2$, at least 10 regions/$cm^2$, at least 25 regions / $cm^2$, at 50 regions / $cm^2$, at least 100 regions / $cm^2$, and at least 200 regions / $cm^2$. For some reactions, lower or mid-range densities may be preferred. For other reactions, higher densities may be suitable. Additionally, even higher densities may be achieved as fabrication technology develops to nano-scale applications.

**[0094]** The number of candidate materials to be included on a physical library is not narrowly critical, and can range, for example, from two to about a million or more, ultimately depending on available fabrication techniques and the nature of the chemical phenomenon or process being investigated. More specifically, the number of different candidate materials incorporated in a library is at least 2, preferably at least 5, more preferably at least 10, still more preferably at least 25, even more preferably at least 50, yet more preferably at least 100, and most preferably at least 250. Present microscale and nanoscale fabrication techniques can be used, however, to prepare arrays having an even greater number of different candidate materials. For higher throughput operations, for example, the number of different candidate materials can be at least about 1000, more preferably at least about 10,000, even more preferably at least about 100,000, and most preferably at least about 1,000,000 or more. The fabrication of arrays comprising very large numbers of different candidate materials is enabled by fabrication techniques known in the integrated circuit arts. *See*, for example, S.M. Sze, Semiconductor Sensors, Chap. 2, pp.17-96, John Wiley & Sons, Inc. (1994). Such approaches have been adapted in other aspects of catalyst research. *See*, for example, Johansson et al., Nanofabrication of Model Catalysts and Simulations of their Reaction Kinetics, J. Vac. Sci. Technol., 17:1 (Jan/Feb 1999).

**[0095]** The invention can be implemented in digital electronic circuitry, or in computer hardware, firmware, software, or in combinations of them. Apparatus of the invention can be implemented in a computer program product tangibly embodied in a machine-readable storage device for execution by a programmable processor; and method steps of the invention can be performed by a programmable processor executing a program of instructions to perform functions of the invention by operating on input data and generating output. The invention can be implemented advantageously in one or more computer programs that are executable on a programmable system including at least one programmable processor coupled to receive data and instructions from, and to transmit data and instructions to, a data storage system, at least one input device, and at least one output device. Each computer program can be implemented in assembly or machine language if desired, or in a high-level procedural or object-oriented programming language, in which case individual design elements can be embodied as data objects in classes having sets of associated properties; in any case, the language can be a compiled or interpreted language. Suitable processors include, by way of example, both general and special purpose microprocessors. Generally, a processor will receive instructions and data from a read-only memory and/or a random access memory. Generally, a computer will include one or more mass storage devices for storing data files; such devices include magnetic disks, such as internal hard disks and removable disks; magneto-optical disks; and optical disks. Storage devices suitable for tangibly embodying computer program instructions and data include all forms of non-volatile memory, including by way of example semiconductor memory devices, such as EPROM, EEPROM, and flash memory devices; magnetic disks such as internal hard disks and removable disks; magneto-optical disks; and CD-ROM disks. Any of the foregoing can be supplemented by, or incorporated in, ASICs (application-specific integrated circuits).

**[0096]** To provide for interaction with a user, the invention can be implemented on a computer system having a display device such as a monitor or LCD screen for displaying information to the user and a keyboard and a pointing device such as a mouse or a trackball by which the user can provide input to the computer system. The computer system can be programmed to provide a graphical user interface through which computer programs interact with users.

**[0097]** The invention has been described in terms of particular embodiments. Other embodiments are within the scope of the following claims. For example, the steps of the invention can be performed in a different order and still achieve desirable results.

## Claims

1. A computer-implemented method (100) for generating a library design for a combinatorial library of materials, a combinatorial library being a collection of two or more members that contain some variance in chemical composition, chemical amount, reaction conditions, and/or processing conditions, a member being a single position in a library, said method being **characterised by**:

   receiving an input defining one or more sources (300) and one or more destinations (310), each source being electronic data representing a component to be used in preparing the combinatorial library and each destination being electronic data representing a conceptual arrangement of cells representing a combinatorial library, the cells corresponding to members of the combinatorial library and/or locations on a physical substrate on which the library will be created;

   receiving an input defining a first mapping (320) the first mapping being electronic data defining a distribution pattern for assigning a component to cells in the arrangement, the distribution pattern including a minimum and a maximum amount of the component to be assigned to any cell of the arrangement and a gradient representing a stepwise change in amount to be applied between the minimum and maximum amounts of the component across the plurality of cells;

   using the first mapping to calculate a composition of one or more materials assigned to one or more of the cells; and

   generating a data file (340) defining the library design, the data file comprising electronic data representing the sources, the destinations and the mapping.

2. The method of claim 1, further comprising:

   displaying a representation of the library design, the representation graphically describing the composition of one or more materials assigned to one or more of the cells.

3. The method of claim 1, wherein the data file comprises electronic data representing one or more sets of properties, each set of properties being associated with one of the sources, the destinations or the mapping.

4. The method of claim 1, wherein defining the sources and destinations comprises receiving an input from a graphical input device.

5. The method of claim 1, wherein the input defining a first mapping comprises a selection from a set of available mapping types, the set of available mapping types comprising a one to one mapping of a component from a source to a cell in the arrangement and a one to many mapping of a component from a source to a plurality of cells in the arrangement.

6. The method of claim 5, wherein the set of available mapping types further comprises a many to many mapping of a plurality of components from a plurality of sources to a plurality of cells in the arrangement.

7. The method of claim 6, wherein the set of available mapping types further comprises a many to one mapping of a plurality of components from a plurality of sources to a cell in the arrangement.

8. The method of claim 5, wherein the set of available mapping types further comprises a set of one or more user-defined equations.

9. The method of claim 1, wherein the gradient is selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression.

10. The method of claim 3, wherein the set of properties associated with the mapping comprises a source name, a source geometry, a destination name, a destination geometry, a gradient type, and a set of gradient parameters defining the gradient.

11. The method of claim 1, further comprising:

receiving an input defining a second mapping, the second mapping being electronic data defining a second distribution pattern for distributing a second component to cells in the arrangement; and

using the first and second mappings to calculate a composition of one or more materials assigned to one or more of the cells.

12. The method of claim 11, wherein the second distribution pattern for assigning a second component includes electronic data identifying a fixed amount of the second component to be assigned to one or more cells in the arrangement.

13. The method of claim 12, wherein the second distribution pattern for assigning a second component includes electronic data identifying a minimum and a maximum amount of the second component to be assigned to any of the cells of the arrangement and a second gradient to be applied between the minimum and maximum amounts of the second component across the cells.

14. The method of claim 1, further comprising generating a modified library design by:

receiving an input redefining a source, a destination or a mapping;

recalculating the composition of one or more materials assigned to one or more of the cells; and

generating a data file defining the modified library design.

15. The method of claim 1, further comprising:

receiving an input defining one or more parameters, each parameter being electronic-data corresponding to a process parameter and defining a parameter value for one or more cells of the arrangement, the parameter value varying between a minimum and a maximum amount; and

wherein the data file further comprises electronic data representing the one or more parameters.

**16.** The method of claim 1, wherein the arrangement comprises two or more cells.

**17.** The method of claim 1, wherein the arrangement comprises ten or more cells.

**18.** The method of claim 1, wherein the arrangement comprises about ninety-six or more cells.

**19.** The method of claim 1, further comprising:

defining a plurality of mappings based in part on the input defining the first mapping, the plurality of mappings in the aggregate defining a composition for each of a plurality of materials assigned to a plurality of cells in the arrangement.

**20.** The method of claim 15, wherein the parameter value is defined to vary over time.

**21.** The method of claim 15, wherein the parameter value is defined to vary across two or more cells in the arrangement.

**22.** The method of claim 15, wherein the parameter value is defined to vary over time and across two or more cells in the arrangement.

**23.** The method of claim 15, wherein the parameter value varies according to a gradient selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression.

**24.** The method of claim 15, wherein the parameter value corresponds to a process parameter selected from the group consisting of temperature, pressure, time, flow rate and stirring speed.

**25.** The method of claim 1, further comprising:

using the data file to cause an automated material handling apparatus to assemble the combinatorial library on a substrate.

**26.** A computer program product on a computer-readable medium for generating a library design for a combinatorial library of materials, a combinatorial library being a collection of two or more members that contain some variance in chemical composition, chemical amount, reaction conditions, and/or processing conditions, a member being a single position in a library, the program being **characterised by** instructions operable to cause a programmable processor to perform all the following steps:

receive an input defining one or more sources (300) and one or more destinations (310), each source being electronic data representing a component to be used in preparing the combinatorial library and each destination being electronic data representing a conceptual arrangement of cells representing a combinatorial library, the cells corresponding to members of the combinatorial library and/or locations on a physical substrate on which the library will be created;

receive an input defining a first mapping (320), the first mapping being electronic data defining a distribution pattern for assigning a component to cells in the arrangement, the distribution pattern including a minimum and a maximum amount of the component to be assigned to any cell of the arrangement anda gradient representing a stepwise change in amount to be applied between the minimum and maximum amounts of the component across the plurality of cells;

use the first mapping to calculate a composition of one or more materials assigned to one or more of the cells; and

generate a data file (340) defining the library design, the data file comprising electronic data representing the sources, the destinations and the mapping.

**27.** The computer program product of claim 26, further comprising instructions operable to cause a programmable processor to:

display a representation of the library design, the representation graphically describing the composition of one or more materials assigned to one or more of the cells.

**28.** The computer program product of claim 26, wherein the data file comprises electronic data representing one or more sets of properties, each set of properties being associated with one of the sources, the destinations or the mapping.

**29.** The computer program product of claim 26, wherein the input defining the sources and destinations comprises an input from a graphical input device.

**30.** The computer program product of claim 26, wherein the input defining a first mapping comprises a selection from a set of available mapping types, the set of available mapping types comprising a one to one mapping of a component from a source to a cell in the arrangement and a one to many mapping of a component from a source to a plurality of cells in the arrangement.

**31.** The computer program product of claim 30, wherein the set of available mapping types further comprises a many to many mapping of a plurality of components from a plurality of sources to a plurality of cells in the arrangement.

**32.** The computer program product of claim 31, wherein the set of available mapping types further comprises a many to one mapping of a plurality of components from a plurality of sources to a cell in the arrangement.

**33.** The computer program product of claim 30, wherein the set of available mapping types further comprises a set of one or more user-defined equations.

**34.** The computer program product of claim 26, wherein the gradient is selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression.

**35.** The computer program product of claim 28, wherein the set of properties associated with the mapping comprises a source name, a source geometry, a destination name, a destination geometry, a gradient type, and a set of gradient parameters defining the gradient.

**36.** The computer program product of claim 26, further comprising instructions operable to cause a programmable processor to:

receive an input defining a second mapping, the second mapping being electronic data defining a second distribution pattern for distributing a second component to cells in the arrangement; and

use the first and second mappings to calculate a composition of one or more materials assigned to one or more of the cells.

**37.** The computer program product of claim 36, wherein the second distribution pattern for assigning a second component includes electronic data identifying a fixed amount of the second component to be assigned to one or more cells in the arrangement.

**38.** The computer program product of claim 37, wherein the second distribution pattern for assigning a second component

includes electronic data identifying a minimum and a maximum amount of the second component to be assigned to any of the cells of the arrangement and a second gradient to be applied between the minimum and maximum amounts of the second component across the cells.

**39.** The computer program product of claim 26, further comprising instructions operable to cause a programmable processor to generate a modified library design by receiving an input redefining a source, a destination or a mapping; recalculating the composition of one or more materials assigned to one or more of the cells; and generating a data file defining the modified library design.

**40.** The computer program product of claim 26, further comprising instructions operable to cause a programmable processor to:

receive an input defining one or more parameters, each parameter being electronic data corresponding to a process parameter and defining a parameter value for one or more cells of the arrangement, the parameter value varying between a minimum and a maximum amount; and

wherein the data file further comprises electronic data representing the one or more parameters.

**41.** The computer program product of claim 26, wherein the arrangement comprises two or more cells.

**42.** The computer program product of claim 26, wherein the arrangement comprises ten or more cells.

**43.** The computer program product of claim 26, wherein the arrangement comprises about ninety-six or more cells.

**44.** The computer program product of claim 26, further comprising instructions operable to cause a programmable processor to:

define a plurality of mappings based in part on the input defining the first mapping, the plurality of mappings in the aggregate defining a composition for each of a plurality of materials assigned to a plurality of cells in the arrangement.

**45.** The computer program product of claim 40, wherein the parameter value is defined to vary over time.

**46.** The computer program product of claim 40, wherein the parameter value is defined to vary across two or more cells in the arrangement.

**47.** The computer program product of claim 40, wherein the parameter value is defined to vary over time and across two or more cells in the arrangement.

**48.** The computer program product of claim 40, wherein the parameter value varies according to a gradient selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression.

**49.** The computer program product of claim 40, wherein the parameter value corresponds to a process parameter selected from the group consisting of temperature, pressure, time, flow rate and stirring speed.

**50.** The computer program product of claim 26, further comprising instructions operable to cause a programmable processor to:

use the data file to cause an automated material handling apparatus to assemble the combinatorial library on a substrate.

**51.** The method of claim 1, wherein

each of the sources has an associated set of source properties describing the source; and

defining the source comprises receiving for each of the sources a set of values for one or more of the source properties associated with the source.

**52.** The method of claim 51, wherein at least one of the source properties is selected from the group consisting of molecular weight, equivalents, density and concentration.

**53.** The method of claim 51, wherein at least one of the source properties is a type describing a class of chemicals to be used in generating the library design.

**54.** The computer program product of claim 26, wherein:

each of the sources has an associated set of source properties describing the source; and

the instructions operable to cause a programmable processor to define the sources include instructions operable to cause a programmable processor to receive for each of the sources a set of values for one or more

of the source properties associated with the source.

55. The computer program product of claim 54, wherein at least one of the source properties is selected from the group consisting of molecular weight, equivalents, density and concentration.

56. The computer program product of claim 54, wherein at least one of the source properties is a type describing a class of chemicals to be used in generating the library design.

**Patentansprüche**

1. Computerimplementiertes Verfahren (100) zum Erzeugen einer Bibliotheksstruktur für eine kombinatorische Bibliothek von Materialien, wobei eine kombinatorische Bibliothek eine Sammlung von zwei oder mehr Elementen ist, die einen gewissen Unterschied hinsichtlich der chemischen Zusammensetzung, der chemischen Menge, der Reaktionsbedingungen und/oder der Prozessbedingungen enthalten, und wobei ein Element eine einzelne Position in einer Bibliothek ist und das Verfahren **gekennzeichnet ist durch**:

   Empfangen einer Eingabe, die eine oder mehrere Quellen (300) und eines oder mehrere Ziele (310) definiert, wobei es sich bei jeder Quelle um elektronische Daten handelt, die eine Komponente darstellen, die bei der Herstellung der kombinatorischen Bibliothek einzusetzen ist, und es sich bei jedem Ziel um elektronische Daten handelt, die eine konzeptionelle Anordnung von Zellen darstellen, die eine kombinatorische Bibliothek darstellt, und wobei die Zellen Elementen der kombinatorischen Bibliothek und/oder Positionen auf einem physischem Substrat entsprechen, auf dem die Bibliothek erzeugt wird;

   Empfangen einer Eingabe, die eine erste Abbildung (320) definiert, wobei es sich bei der ersten Abbildung um elektronische Daten handelt, die ein Verteilungsmuster zum Zuordnen einer Komponente zu Zellen in der Anordnung definieren, und wobei das Verteilungsmuster eine minimale und eine maximale Menge der Komponente, die jeder beliebigen Zelle der Anordnung zuzuordnen sind, sowie einen Gradienten enthält, der eine schrittweise Änderung der Menge darstellt, die zwischen der minimalen und der maximalen Menge der Komponente über die Vielzahl von Zellen anzuwenden ist;

   Einsetzen der ersten Abbildung, um eine Zusammensetzung eines Materials oder mehrerer Materialien zu errechnen, die einer oder mehreren der Zellen zugeordnet ist, und

   Erzeugen einer Datendatei (340), die die Bibliotheksstruktur definiert, wobei die Datendatei elektronische Daten umfasst, die die Quellen, die Ziele und die Abbildung darstellen.

2. Verfahren nach Anspruch 1, das des Weiteren umfasst:

   Anzeigen einer Darstellung der Bibliotheksstruktur, wobei die Darstellung grafisch die Zusammensetzung eines Materials oder mehrerer Materialien beschreibt, die einer oder mehreren der Zellen zugeordnet ist.

3. Verfahren nach Anspruch 1, wobei die Datendatei elektronische Daten umfasst, die eine oder mehrere Gruppen von Eigenschaften darstellen, wobei jede Gruppe von Eigenschaften mit den Quellen, den Zielen oder der Abbildung verbunden ist.

4. Verfahren nach Anspruch 1, wobei das Definieren der Quellen und der Ziele das Empfangen einer Eingabe von einer grafischen Eingabevorrichtung umfasst.

5. Verfahren nach Anspruch 1, wobei die Eingabe, die eine erste Abbildung definiert, eine Auswahl aus einer Gruppe zur Verfügung stehender Abbildungstypen umfasst, wobei die Gruppe zur Verfügung stehender Abbildungstypen eine eindeutige Abbildung einer Komponente von einer Quelle auf einer Zelle in der Anordnung und eine mehrdeutige Abbildung einer Komponente von einer Quelle auf einer Vielzahl von Zellen in der Anordnung umfasst.

6. Verfahren nach Anspruch 5, wobei die Gruppe zur Verfügung stehender Abbildungstypen des Weiteren eine mehrmehrdeutige Abbildung einer Vielzahl von Komponenten von einer Vielzahl von Quellen auf einer Vielzahl von Zellen in der Anordnung umfasst.

7. Verfahren nach Anspruch 6, wobei die Gruppe zur Verfügung stehender Abbildungstypen des Weiteren eine nacheindeutige Abbildung einer Vielzahl von Komponenten von einer Vielzahl von Quellen auf einer Zelle in der Anordnung umfasst.

8. Verfahren nach Anspruch 5, wobei die Gruppe zur Verfügung stehender Abbildungstypen des Weiteren eine Gruppe einer oder mehrerer benutzerdefinierter Gleichungen umfasst.

9. Verfahren nach Anspruch 1, wobei der Gradient aus der Gruppe ausgewählt wird, die aus linearer, logarithmischer, exponentialer, polynomialer und geometrischer Progression besteht.

10. Verfahren nach Anspruch 3, wobei die Gruppe von Eigenschaften, die mit der Abbildung verbunden ist, einen Quellennamen, eine Quellengeometrie, einen Zielnamen, eine Zielgeometrie, einen Gradiententyp und eine Gruppe von Gradientenparametern, die den Gradienten definieren, umfasst.

11. Verfahren nach Anspruch 1, das des Weiteren umfasst:

Empfangen einer Eingabe, die eine zweite Abbildung definiert, wobei es sich bei der zweiten Abbildung um elektronische Daten handelt, die ein zweites Verteilungsmuster zum Verteilen einer zweiten Komponente auf Zellen in der Anordnung definieren; und

Einsetzen der ersten und der zweiten Abbildung, um eine Zusammensetzung eines Materials oder mehrerer Materialien zu errechnen, die einer oder mehreren der Zellen zugeordnet sind.

12. Verfahren nach Anspruch 11, wobei das zweite Verteilungsmuster zum Zuordnen einer zweiten Komponente elektronische Daten enthält, die eine unveränderliche Menge der zweiten Komponente angeben, die einer oder mehreren Zellen in der Anordnung zuzuordnen ist.

13. Verfahren nach Anspruch 12, wobei das zweite Verteilungsmuster zum Zuordnen einer zweiten Komponente elektronische Daten enthält, die eine minimale und eine maximale Menge der zweiten Komponente, die jeder beliebigen der Zellen der Anordnung zuzuordnen sind, und einen zweiten Gradienten angeben, der zwischen der minimalen und der maximalen Menge der zweiten Komponente über die Zellen anzuwenden ist.

14. Verfahren nach Anspruch 1, das des Weiteren das Erzeugen einer modifizierten Bibliotheksstruktur durch die folgenden Schritte umfasst:

Empfangen einer Eingabe, die eine Quelle, ein Ziel oder eine Abbildung neu definiert;

erneutes Errechnen der Zusammensetzung eines Materials oder mehrerer Materialien, die einer oder mehreren der Zellen zugeordnet sind; und

Erzeugen einer Datendatei, die die modifizierte Bibliotheksstruktur definiert.

15. Verfahren nach Anspruch 1, das des Weiteren umfasst:

Empfangen einer Eingabe, die einen oder mehrere Parameter definiert, wobei es sich bei jedem Parameter um elektronische Daten handelt, die einem Prozessparameter entsprechen und einen Parameterwert für eine oder mehrere Zellen der Anordnung definieren, wobei der Parameterwert zwischen einem minimalen und einem maximalen Betrag variiert; und

wobei die Datendatei des Weiteren elektronische Daten umfasst, die den einen oder die mehreren Parameter darstellen.

16. Verfahren nach Anspruch 1, wobei die Anordnung zwei oder mehr Zellen umfasst.

17. Verfahren nach Anspruch 1, wobei die Anordnung 10 oder mehr Zellen umfasst.

18. Verfahren nach Anspruch 1, wobei die Anordnung ungefähr 96 oder mehr Zellen umfasst.

19. Verfahren nach Anspruch 1, das des Weiteren umfasst:

Definieren einer Vielzahl von Abbildungen, die teilweise auf der Eingabe beruhen, die die erste Abbildung definiert, wobei die Vielzahl von Abbildungen in dem Aggregat eine Zusammensetzung für jedes einer Vielzahl von Materialien definiert, die einer Vielzahl von Zellen in der Anordnung zugeordnet ist.

20. Verfahren nach Anspruch 15, wobei der Parameterwert so definiert ist, dass er mit der Zeit variiert.

21. Verfahren nach Anspruch 15, wobei der Parameterwert so definiert ist, dass er über zwei oder mehr Zellen in der Anordnung variiert.

22. Verfahren nach Anspruch 15, wobei der Parameterwert so definiert ist, dass er mit der Zeit und über zwei oder mehr Zellen in der Anordnung variiert.

23. Verfahren nach Anspruch 15, wobei der Parameterwert entsprechend einem Gradienten variiert, der aus der Gruppe ausgewählt wird, die aus linearer, logarithmischer, exponentialer, polynomialer und geometrischer Progression besteht.

24. Verfahren nach Anspruch 15, wobei der Parameterwert einem Prozessparameter entspricht, der aus der Gruppe ausgewählt wird, die aus Temperatur, Druck, Zeit, Strömungsmenge und Rührgeschwindigkeit besteht.

25. Verfahren nach Anspruch 1, das des Weiteren umfasst:

Einsatz der Datendatei, um damit zu bewirken, dass eine automatische Materialhandhabungsvorrichtung die kombinatorische Bibliothek auf einem Substrat zusammenstellt.

26. Computerprogrammerzeugnis auf einem computerlesbaren Medium zu Erzeugen einer Bibliotheksstruktur für eine kombinatorische Bibliothek von Materialien, wobei eine kombinatorische Bibliothek eine Sammlung von zwei oder mehr Elementen ist, die einen gewissen Unterschied der chemischen Zusammensetzung, der chemischen Menge, der Reaktionsbedingungen und/oder der Prozessbedingungen enthalten, und wobei ein Element eine einzelne Position in einer Bibliothek ist und das Programm durch Befehle **gekennzeichnet** ist, die ausgeführt werden können, um einen programmierbaren Prozessor zu veranlassen, alle folgenden Schritte auszuführen:

Empfangen einer Eingabe, die eine oder mehrere Quellen (300) und eines oder mehrere Ziele (310) definiert, wobei es sich bei jeder Quelle um elektronische Daten handelt, die eine Komponente darstellen, die bei der Herstellung der kombinatorischen Bibliothek einzusetzen ist, und es sich bei jedem Ziel um elektronische Daten handelt, die eine konzeptionelle Anordnung von Zellen darstellen, die eine kombinatorische Bibliothek darstellt, wobei die Zellen Elementen der kombinatorischen Bibliothek und/oder Positionen auf einem physischen Substrat entsprechen, auf dem die Bibliothek erzeugt wird;

Empfangen einer Eingabe, die eine erste Abbildung (320) definiert, wobei es sich bei der ersten Abbildung um elektronische Daten handelt, die ein Verteilungsmuster zum Zuordnen einer Komponente zu Zellen in der Anordnung definieren, und wobei das Verteilungsmuster eine minimale und eine maximale Menge der Komponente, die jeder beliebigen Zelle der Anordnung zuzuordnen sind, sowie einen Gradienten enthält, der eine schrittweise Änderung der Menge darstellt, die zwischen der minimalen und der maximalen Menge der Komponente über die Vielzahl von Zellen anzuwenden ist;

Einsetzen der ersten Abbildung um eine Zusammensetzung eines Materials oder mehrere Materialien zu errechnen, die einer oder mehreren der Zellen zugeordnet sind; und

Erzeugen einer Datendatei (340), die die Bibliotheksstruktur definiert, wobei die Datendatei elektronische Daten umfasst, die die Quellen, die Ziele und die Abbildungen darstellen.

27. Computerprogrammerzeugnis nach Anspruch 26, das des Weiteren Befehle umfasst, die ausgeführt werden können, um einen programmierbaren Prozessor zu folgendem zu veranlassen:

Anzeigen einer Darstellung der Bibliotheksstruktur, wobei die Bibliotheksstruktur grafisch die Zusammensetzung eines Materials oder mehrerer Materialien beschreibt, die einer oder mehreren der Zellen zugeordnet ist.

28. Computerprogrammerzeugnis nach Anspruch 26, wobei die Datendatei elektronische Daten umfasst, die eine oder mehrere Gruppen von Eigenschaften darstellen, wobei jede Gruppe von Eigenschaften mit den Quellen, den Zielen oder der Abbildung verbunden ist.

29. Computerprogrammerzeugnis nach Anspruch 26, wobei die Eingabe, die die Quellen und die Ziele definiert, eine Eingabe von einer grafischen Eingabevorrichtung umfasst.

30. Computerprogrammerzeugnis nach Anspruch 26, wobei die Eingabe, die eine erste Abbildung definiert, eine Auswahl aus einer Gruppe zur Verfügung stehender Abbildungstypen umfasst, wobei die Gruppe zur Verfügung stehender Abbildungstypen eine eindeutige Abbildung einer Komponente von einer Quelle auf einer Zelle in der Anordnung und eine mehrdeutige Abbildung einer Komponente von einer Quelle auf einer Vielzahl von Zellen in der Anordnung umfasst.

31. Computerprogrammerzeugnis nach Anspruch 30, wobei die Gruppe zur Verfügung stehender Abbildungstypen des Weiteren eine mehrmehrdeutige Abbildung einer Vielzahl von Komponenten von einer Vielzahl von Quellen auf einer Vielzahl von Zellen in der Anordnung umfasst.

32. Computerprogrammerzeugnis nach Anspruch 31, wobei die Gruppe zur Verfügung stehender Abbildungstypen des Weiteren eine nacheindeutige Abbildung einer Vielzahl von Komponenten von einer Vielzahl von Quellen auf einer Zelle in der Anordnung umfasst.

33. Computerprogrammerzeugnis nach Anspruch 30, wobei die Gruppe zur Verfügung stehender Abbildungstypen des Weiteren eine Gruppe einer oder mehrerer benutzerdefinierter Gleichungen umfasst.

34. Computerprogrammerzeugnis nach Anspruch 26, wobei der Gradient aus der Gruppe ausgewählt wird, die aus linearer, logarithmischer, exponentialer, polynomialer und geometrischer Progression besteht.

35. Computerprogrammerzeugnis nach Anspruch 28, wobei die Gruppe von Eigenschaften, die mit der Abbildung verbunden ist, einen Quellennamen, eine Quellengeometrie, einen Zielnamen, eine Zielgeometrie, einen Gradiententyp und eine Gruppe von Gradientenparametem, die den Gradienten definieren, umfasst.

36. Computerprogrammerzeugnis nach Anspruch 26, das des Weiteren Befehle umfasst, die ausgeführt werden können, um einen Computer zu folgendem zu veranlassen:

    Empfangen einer Eingabe, die eine zweite Abbildung definiert, wobei es sich bei der zweiten Abbildung um elektronische Daten handelt, die ein zweites Verteilungsmuster zum Verteilen einer zweiten Komponente auf Zellen in der Anordnung definieren; und

    Einsetzen der ersten und der zweiten Abbildung, um eine Zusammensetzung eines Materials oder mehrerer Materialien zu errechnen, die einer oder mehreren der Zellen in der Anordnung zugeordnet sind.

37. Computerprogrammerzeugnis nach Anspruch 36, wobei das zweite Verteilungsmuster zum Zuordnen einer zweiten Komponente elektronische Daten enthält, die eine unveränderliche Menge der zweiten Komponente angeben, die einer oder mehreren Zellen in der Anordnung zuzuordnen ist.

38. Computerprogrammerzeugnis nach Anspruch 37, wobei das zweite Verteilungsmuster zum Zuordnen einer zweiten Komponente elektronische Daten enthält, die eine minimale und eine maximale Menge der zweiten Komponente, die jeder beliebigen der Zellen der Anordnung zuzuordnen sind, und einen zweiten Gradienten angeben, der zwischen der minimalen und der maximalen Menge der zweiten Komponente über die Zellen anzuwenden ist.

39. Computerprogrammerzeugnis nach Anspruch 26, das des Weiteren Befehle umfasst, die ausgeführt werden können, um zu bewirken, dass ein programmierbarer Prozessor eine modifizierte Bibliotheksstruktur erzeugt, indem er eine Eingabe empfängt, die eine Quelle, ein Ziel oder eine Abbildung neu definiert, die Zusammensetzung eines Materials oder mehrerer Materialien erneut errechnet, die einer oder mehreren der Zellen zugeordnet sind; und eine Datendatei erzeugt, die die modifizierte Bibliotheksstruktur definiert.

40. Computerprogrammerzeugnis nach Anspruch 26, das des Weiteren Befehle umfasst, die ausgeführt werden können, um einen programmierbaren Prozessor zu folgendem zu veranlassen:

Empfangen einer Eingabe, die einen oder mehrere Parameter definiert, wobei es sich bei jedem Parameter um elektronische Daten handelt, die einem Prozessparameter entsprechen und einen Parameterwert für eine oder mehrere Zellen der Anordnung definieren, wobei der Parameterwert zwischen einem minimalen und einem maximalen Betrag variiert; und

wobei die Datendatei des Weiteren elektronische Daten umfasst, die den einen oder die mehreren Parameter darstellen.

41. Computerprogrammerzeugnis nach Anspruch 26, wobei die Anordnung zwei oder mehr Zellen umfasst.

42. Computerprogrammerzeugnis nach Anspruch 26, wobei die Anordnung 10 oder mehr Zellen umfasst.

43. Computerprogrammerzeugnis nach Anspruch 26, wobei die Anordnung ungefähr 96 oder mehr Zellen umfasst.

44. Computerprogrammerzeugnis nach Anspruch 26, die des Weiteren Befehle umfasst, die ausgeführt werden können, um einen Computer zu folgendem zu veranlassen:

Definieren einer Vielzahl von Abbildungen, die teilweise auf der Eingabe beruhen, die die erste Abbildung definiert, wobei die Vielzahl von Abbildungen in dem Aggregat eine Zusammensetzung für jedes einer Vielzahl von Materialien definiert, die einer Vielzahl von Zellen in der Anordnung zugeordnet ist.

45. Computerprogrammerzeugnis nach Anspruch 40, wobei der Parameterwert so definiert ist, dass er mit der Zeit variiert.

46. Computerprogrammerzeugnis nach Anspruch 40, wobei der Parameterwert so definiert ist, dass er über zwei oder mehr Zellen in der Anordnung variiert.

47. Computerprogrammerzeugnis nach Anspruch 40, wobei der Parameterwert so definiert ist, dass er mit der Zeit und über zwei oder mehr Zellen in der Anordnung variiert.

48. Computerprogrammerzeugnis nach Anspruch 40, wobei der Parameterwert entsprechend einem Gradienten variiert, der aus der Gruppe ausgewählt wird, die aus linearer, logarithmischer, exponentialer, polynomialer und geometrischer Progression besteht.

49. Computerprogrammerzeugnis nach Anspruch 40, wobei der Parameterwert einem Prozessparameter entspricht, der aus der Gruppe ausgewählt wird, die aus Temperatur, Druck, Strömungsmenge und Rührgeschwindigkeit besteht.

50. Computerprogrammerzeugnis nach Anspruch 26, das des Weiteren Befehle umfasst, die ausgeführt werden können, um einen Computer zu folgendem zu veranlassen:

Einsatz der Datendatei, um eine automatisierte Materialhandhabungsvorrichtung zu veranlassen, die kombinatorische Bibliothek auf einem Substrat zusammenzustellen.

51. Verfahren nach Anspruch 1, wobei:

jede der Quellen eine damit verbundene Gruppe von Quelleneigenschaften aufweist, die die Quelle beschreiben; und

Definieren der Quelle Empfangen einer Gruppe von Werten für eine oder mehrere der Quelleneigenschaften, die mit der Quelle verbunden sind, für jede der Quellen umfasst.

52. Verfahren nach Anspruch 51, wobei wenigstens eine der Quelleneigenschaften aus der Gruppe ausgewählt wird, die aus Molekulargewicht, Äquivalenten, Dichte und Konzentration besteht.

53. Verfahren nach Anspruch 51, wobei wenigstens eine der Quelleneigenschaften ein Typ ist, der eine Klasse von Chemikalien beschreibt, die beim Erzeugen der Bibliotheksstruktur einzusetzen sind.

54. Computerprogrammerzeugnis nach Anspruch 26, wobei:

jede der Quellen eine damit verbundene Gruppe von Quelleneigenschaften aufweist, die die Quelle beschreiben; und

die Befehle, die ausgeführt werden können, um einen Computer zu veranlassen, die Quellen zu definieren, Befehle einschließen, die ausgeführt werden können, um einen programmierbaren Prozessor zu veranlassen, für jede der Quellen eine Gruppe von Werten für eine oder mehrere der Quelleneigenschaften zu empfangen, die mit der Quelle verbunden sind.

55. Computerprogrammerzeugnis nach Anspruch 54, wobei wenigstens eine der Quelleneigenschaften aus der Gruppe ausgewählt wird, die aus Molekulargewicht, Äquivalenten, Dichte und Konzentration bestehen.

56. Computerprogrammerzeugnis nach Anspruch 54, wobei wenigstens eine der Quelleneigenschaften ein Typ ist, der eine Klasse von Chemikalien beschreibt, die beim Erzeugen der Bibliotheksstruktur einzusetzen sind.

**Revendications**

1. Procédé mis en oeuvre sur ordinateur (100) pour générer un concept de bibliothèque destiné à une bibliothèque combinatoire de matériaux, une bibliothèque combinatoire étant une collection de deux éléments ou plus présentant une certaine variance de composition chimique, de quantité de composé chimique, de conditions réactionnelles, et/ou de conditions de traitement, un élément étant une position unique dans une bibliothèque, ledit procédé étant **caractérisé par** le fait de :

recevoir une entrée définissant une ou plusieurs sources (300) et une ou plusieurs destinations (310), chaque source étant constituée de données électroniques représentant un constituant à utiliser dans la préparation de la bibliothèque combinatoire et chaque destination étant constituée de données électroniques représentant une configuration conceptuelle de cellules représentant une bibliothèque combinatoire et/ou des positions sur un substrat physique sur lequel sera créée la bibliothèque ;
recevoir une entrée définissant une première projection (320), la première projection étant constituée de données électroniques définissant un diagramme de distribution destiné à affecter un constituant à des cellules de la configuration, le diagramme de distribution comprenant des quantités minimum et maximum du constituant devant être affecté à toute cellule de l'agencement et un gradient représentant une modification graduelle de la quantité à appliquer entre les quantités minimum et maximum du constituant parmi la pluralité de cellules ;
utiliser la première projection pour calculer une composition d'un ou de plusieurs matériaux affectés à une ou plusieurs des cellules ; et
créer un fichier de données (340) définissant le concept de bibliothèque, le fichier de données comprenant des données électroniques représentant les sources, les destinations et la projection.

2. Procédé selon la revendication 1, consistant en outre à :

afficher une représentation du concept de bibliothèque, la représentation décrivant graphiquement la composition d'un ou plusieurs matériaux affectés à une ou plusieurs des cellules.

3. Procédé selon la revendication 1, dans lequel le fichier de données comprend des données électroniques représentant un ou plusieurs ensembles de propriétés, chaque ensemble de propriétés étant associé à l'une des sources, des destinations ou de la projection.

4. Procédé selon la revendication 1, dans lequel la définition des sources et des destinations consiste à recevoir une entrée d'un dispositif d'entrée graphique.

5. Procédé selon la revendication 1, dans lequel l'entrée définissant une première projection comprend une sélection parmi un ensemble de types de projections disponibles, l'ensemble de types de projections disponibles comprenant une projection à origine unique et à destination unique d'un constituant depuis une source vers une cellule de la configuration et une projection à origine unique et à destinations multiples d'un constituant, depuis une source vers une pluralité de cellules de la configuration.

6. Procédé selon la revendication 5, dans lequel l'ensemble de types de projections disponibles comprend en outre une projection d'origines multiples vers des destinations multiples d'une pluralité de constituants depuis une pluralité de sources vers une pluralité de cellules de la configuration.

7. Procédé selon la revendication 6, dans lequel l'ensemble de types de projections disponibles comprend en outre une projection d'origines multiples vers une destination unique d'une pluralité de constituants depuis une pluralité de sources vers une cellule de la configuration.

8. Procédé selon la revendication 5, dans lequel l'ensemble de types de projections disponibles comprend en outre un ensemble d'une ou plusieurs équations définies par l'utilisateur.

9. Procédé selon la revendication 1, dans lequel le gradient est sélectionné dans le groupe constitué de progressions linéaire, logarithmique, exponentielle, polynomiale et géométrique.

10. Procédé selon la revendication 3, dans lequel l'ensemble de propriétés associées à la projection comprend un nom de source, une géométrie de source, un nom de destination, une géométrie de destination, un type de gradient, et un ensemble de paramètres de gradient définissant le gradient.

11. Procédé selon la revendication 1, consistant en outre à :

recevoir une entrée définissant une seconde projection, la seconde projection étant constituée de données électroniques définissant un second diagramme de distribution pour la distribution d'un second constituant vers des cellules de la configuration ; et
utiliser les première et seconde projections pour calculer une composition d'un ou plusieurs matériaux affectés à une ou plusieurs des cellules.

12. Procédé selon la revendication 11, dans lequel le second diagramme de distribution destiné à l'affectation d'un second constituant contient des données électroniques identifiant une quantité fixe du second constituant devant être affecté à une ou plusieurs cellules de la configuration.

13. Procédé selon la revendication 12, dans lequel le second diagramme de distribution destiné à affecter un second constituant contient des données électroniques identifiant des quantités minimum et maximum du second constituant devant être affecté à l'une quelconque des cellules de la configuration et un second gradient devant être appliqué entre les quantités minimum et maximum du second constituant parmi toutes les cellules.

14. Procédé selon la revendication 1, consistant en outre à créer un concept de bibliothèque modifié par le fait de :

recevoir une entrée redéfinissant une source, une destination ou une projection ;
recalculer la composition d'un ou plusieurs matériaux affectés à une ou plusieurs des cellules ; et
créer un fichier de données définissant le concept de bibliothèque modifié.

15. Procédé selon la revendication 1, consistant en outre à :

recevoir une entrée définissant un ou plusieurs paramètres, chaque paramètre étant constitué de données électroniques correspondant à un paramètre de traitement et définissant une valeur de paramètre pour une ou plusieurs cellules de la configuration, la valeur du paramètre variant entre des quantités minimum et maximum ; et
dans lequel le fichier de données comprend en outre des données électroniques représentant ces un ou plusieurs paramètres.

16. Procédé selon la revendication 1, dans lequel la configuration comprend deux cellules ou davantage.

17. Procédé selon la revendication 1, dans lequel la configuration comprend dix cellules ou davantage.

18. Procédé selon la revendication 1, dans lequel la configuration comprend environ quatre-vingt seize cellules ou davantage.

19. Procédé selon la revendication 1, consistant en outre à :

définir une pluralité de projections fondées en partie sur l'entrée définissant la première projection, la pluralité de projections contenues dans l'agrégat définissant une composition pour chacun d'une pluralité de matériaux affectés à une pluralité de cellules de la configuration.

**20.** Procédé selon la revendication 15, dans lequel la valeur du paramètre est définie de façon à varier au cours du temps.

**21.** Procédé selon la revendication 15, dans lequel la valeur du paramètre est définie de façon à varier parmi deux cellules ou davantage de la configuration.

**22.** Procédé selon la revendication 15, dans lequel la valeur du paramètre est définie de façon à varier au cours du temps et dans deux cellules ou davantage de la configuration.

**23.** Procédé selon la revendication 15, dans lequel la valeur du paramètre varie en fonction du gradient sélectionné dans le groupe constitué de progressions linéaire, logarithmique, exponentielle, polynomiale et géométrique.

**24.** Procédé selon la revendication 15, dans lequel la valeur du paramètre correspond à un paramètre de traitement sélectionné dans le groupe constitué de la température, de la pression, du temps, du débit et de la vitesse d'agitation.

**25.** Procédé selon la revendication 1, consistant en outre à :

utiliser le fichier de données pour faire en sorte que l'appareil de manipulation automatique de matériau assemble la bibliothèque combinatoire sur un substrat.

**26.** Produit à programme informatique stocké sur un support lisible par ordinateur pour générer un concept de bibliothèque pour une bibliothèque combinatoire de matériaux, une bibliothèque combinatoire étant une collection de deux éléments ou davantage qui présentent une certaine variance de composition chimique, de quantité de composé chimique, de conditions réactionnelles, et/ou de conditions de traitement, un élément étant une position unique dans une bibliothèque, le programme étant **caractérisé par** des instructions ayant pour fonction de faire en sorte qu'un processeur programmable effectue la totalité des étapes suivantes :

recevoir une entrée définissant une ou plusieurs sources (300) et une ou plusieurs destinations (310), chaque source étant constituée de données électroniques représentant un constituant devant être utilisé dans la préparation de la bibliothèque combinatoire et chaque destination étant constituée de données électroniques représentant une configuration conceptuelle de cellules représentant une bibliothèque combinatoire, les cellules correspondant à des éléments de la bibliothèque combinatoire et/ou à des positions sur un substrat physique sur lequel sera créée la bibliothèque ;
recevoir une entrée définissant une première projection (320), la première projection étant constituée de données électroniques définissant un diagramme de distribution permettant d'affecter un constituant à des cellules de la configuration, le diagramme de distribution comprenant des quantités minimum et maximum du constituant devant être affecté à une cellule quelconque de la configuration et un gradient représentant une variation graduelle de la quantité devant être appliquée entre les quantités minimum et maximum du constituant dans la pluralité de cellules ;
utiliser la première projection pour calculer une composition d'un ou de plusieurs matériaux affectés à une ou plusieurs des cellules ; et
créer un fichier de données (340) définissant le concept de bibliothèque, le fichier de données comprenant des données électroniques représentant les sources, les destinations et la projection.

**27.** Produit à programme informatique selon la revendication 26, comprenant en outre des instructions ayant pour fonction de faire en sorte qu'un processeur programmable :

affiche une représentation du concept de bibliothèque, la représentation décrivant graphiquement la composition d'un ou plusieurs matériaux affectés à une ou plusieurs des cellules.

**28.** Produit à programme informatique selon la revendication 26, dans lequel le fichier de données comprend des données électroniques représentant un ou plusieurs ensembles de propriétés, chaque ensemble de propriétés étant associé à l'une des sources, des destinations ou de la projection.

29. Produit à programme informatique selon la revendication 26, dans lequel l'entrée définissant les sources et les destinations comprend une entrée fournie par un dispositif d'entrée graphique.

30. Produit à programme informatique selon la revendication 26, dans lequel l'entrée définissant une première projection comprend une sélection parmi un ensemble de types de projections disponibles, l'ensemble de types de projections disponibles comprenant une projection à origine unique et à destination unique depuis une source vers une cellule de la configuration et une projection à origine unique et à destinations multiples d'un constituant, depuis une source vers une pluralité de cellules de la configuration.

31. Produit à programme informatique selon la revendication 30, dans lequel l'ensemble de types de projections disponibles comprend en outre une projection à origines multiples et à destinations multiples d'une pluralité de constituants depuis une pluralité de sources vers une pluralité de cellules de la configuration.

32. Produit à programme informatique selon la revendication 31, dans lequel l'ensemble de types de projections disponibles comprend en outre une projection à origines multiples et à destination unique d'une pluralité de constituants depuis une pluralité de sources vers une cellule de la configuration.

33. Produit à programme informatique selon la revendication 30, dans lequel l'ensemble de types de projections disponibles comprend en outre un ensemble d'une ou plusieurs équations définies par l'utilisateur.

34. Produit à programme informatique selon la revendication 26, dans lequel le gradient est sélectionné dans le groupe constitué de progressions linéaire, logarithmique, exponentielle, polynomiale et géométrique.

35. Produit à programme informatique selon la revendication 28, dans lequel l'ensemble de propriétés associées à la projection comprend un nom de source, une géométrie de la source, un nom de destination, une géométrie de la destination, un type de gradient, et un ensemble de paramètres de gradient définissant le gradient.

36. Produit à programme informatique selon la revendication 26, comprenant en outre des instructions ayant pour fonction de faire en sorte qu'un processeur programmable :

reçoive une entrée définissant une seconde projection, la seconde projection étant constituée de données électroniques définissant un second diagramme de distribution destiné à distribuer un second constituant à des cellules de la configuration ; et
utilise les première et seconde projections pour calculer une composition d'un ou plusieurs matériaux affectés à une ou plusieurs des cellules.

37. Produit à programme informatique selon la revendication 36, dans lequel le second diagramme de distribution destiné à affecter un second constituant contient des données électroniques identifiant une quantité fixe du second constituant devant être affecté à une ou plusieurs cellules de la configuration.

38. Produit à programme informatique selon la revendication 37, dans lequel le second diagramme de distribution destiné à affecter un second constituant

contient des données électroniques identifiant des quantités minimum et maximum du second constituant devant être affecté à l'une quelconque des cellules de la configuration et un second gradient devant être appliqué entre les quantités minimum et maximum du second constituant dans les cellules.

39. Produit à programme informatique selon la revendication 26, comprenant en outre des instructions ayant pour fonction de faire en sorte qu'un processeur programmable génère un concept de bibliothèque modifié en recevant une entrée redéfinissant une source, une destination ou un projection, recalcule la composition d'un ou plusieurs matériaux affectés à une ou plusieurs des cellules, et génère un fichier de données définissant le concept de bibliothèque modifié.

40. Produit à programme informatique selon la revendication 26, comprenant en outre des instructions ayant pour fonction de faire en sorte qu'un processeur programmable :

reçoive une entrée définissant un ou plusieurs paramètres, chaque paramètre étant constitué de données électroniques correspondant à un paramètre de traitement et définissant une valeur de paramètre pour une

ou plusieurs cellules de la configuration, la valeur du paramètre variant entre des quantités minimum et maximum ; et
dans lequel le fichier de données comprend en outre des données électroniques représentant un ou plusieurs paramètres.

**41.** Produit à programme informatique selon la revendication 26, dans lequel la configuration comprend deux cellules ou davantage.

**42.** Produit à programme informatique selon la revendication 26, dans lequel la configuration comprend dix cellules ou davantage.

**43.** Produit à programme informatique selon la revendication 26, dans lequel la configuration comprend environ quatre-vingt seize cellules ou davantage.

**44.** Produit à programme informatique selon la revendication 26, comprenant en outre des instructions ayant pour effet de faire en sorte qu'un processeur programmable :

définisse une pluralité de projections fondées en partie sur l'entrée définissant la première projection, la pluralité de projections de l'agrégat définissant une composition pour chacun d'une pluralité de matériaux affectés à une pluralité de cellules de la configuration.

**45.** Produit à programme informatique selon la revendication 40, dans lequel la valeur du paramètre est définie de façon à varier au cours du temps.

**46.** Produit à programme informatique selon la revendication 40, dans lequel la valeur du paramètre est définie de façon à varier parmi deux cellules ou davantage de la configuration.

**47.** Produit à programme informatique selon la revendication 40, dans lequel la valeur du paramètre est définie de façon à varier au cours du temps et parmi deux cellules ou davantage de la configuration.

**48.** Produit à programme informatique selon la revendication 40, dans lequel la valeur du paramètre varie conformément à un gradient sélectionné dans le groupe constitué de progressions linéaire, logarithmique, exponentielle, polynomiale et géométrique.

**49.** Produit à programme informatique selon la revendication 40, dans lequel la valeur du paramètre correspond à un paramètre de traitement sélectionné dans le groupe constitué de la température, de la pression, du temps, du débit et de la vitesse d'agitation.

**50.** Produit à programme informatique selon la revendication 26, comprenant en outre des instructions ayant pour fonction de faire en sorte qu'un processeur programmable :

utilise le fichier de données pour faire en sorte qu'un appareil de manipulation automatique de matériau assemble la bibliothèque combinatoire sur un substrat.

**51.** Procédé selon la revendication 1, dans lequel :

chacune des sources comporte un ensemble associé de propriétés de sources décrivant la source ; et
la définition de la source consiste à recevoir pour chacune des sources un ensemble de valeurs pour une ou plusieurs des propriétés de la source qui sont associées à la source.

**52.** Procédé selon la revendication 51, dans lequel au moins l'une des propriétés de la source est sélectionnée dans le groupe constitué de la masse moléculaire, des équivalents de la densité et de la concentration.

**53.** Procédé selon la revendication 51, dans lequel au moins l'une des propriétés de la source est un type décrivant une classe de composés chimiques devant être utilisés pour créer le concept de bibliothèque.

**54.** Produit à programme informatique selon la revendication 26, dans lequel :

chacune des sources comporte un ensemble associé de propriétés de source décrivant la source ; et
les instructions ayant pour fonction de faire en sorte qu'un processeur programmable définisse les sources comprennent des instructions ayant pour fonction de faire en sorte qu'un processeur programmable reçoive pour chacune des sources un ensemble de valeurs pour une ou plusieurs des propriétés de la source qui sont associées à la source.

**55.** Produit à programme informatique selon la revendication 54, dans lequel au moins l'une des propriétés de la source est sélectionnée dans le groupe constitué de la masse moléculaire, d'équivalents, de la densité et de la concentration.

**56.** Produit à programme informatique selon la revendication 54, dans lequel au moins l'une des propriétés de la source est un type décrivant une classe de composés chimiques devant être utilisés pour générer le concept de bibliothèque.

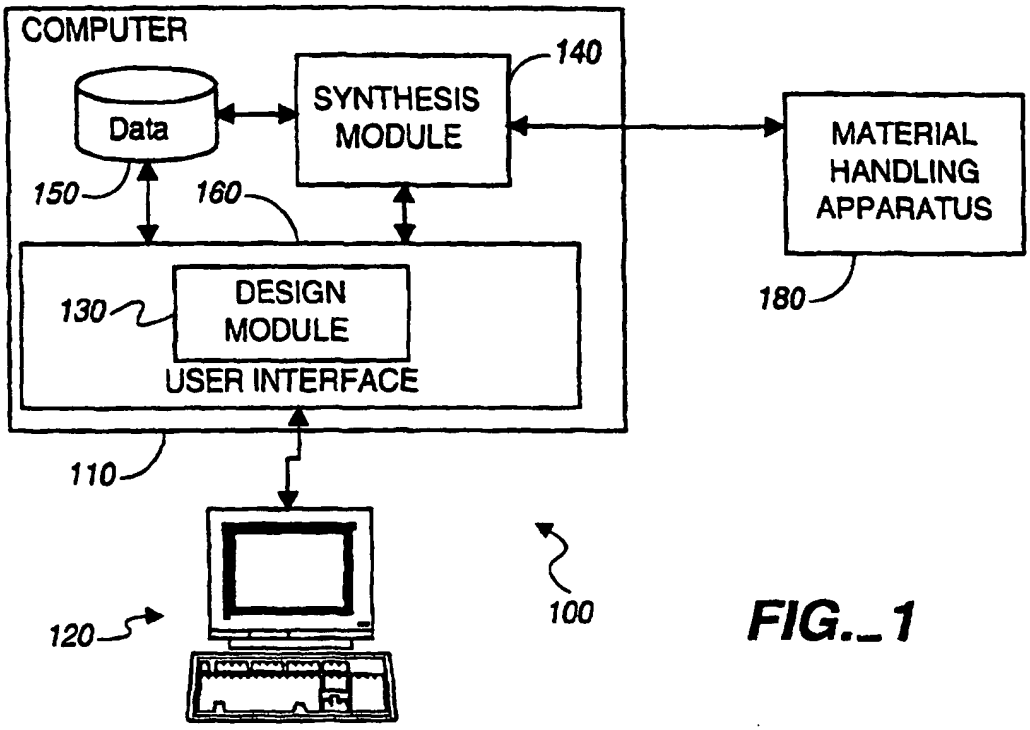

COMPUTER
Data
SYNTHESIS MODULE
140
MATERIAL HANDLING APPARATUS
150
160
DESIGN MODULE
130
USER INTERFACE
180
110
120
100

FIG._1

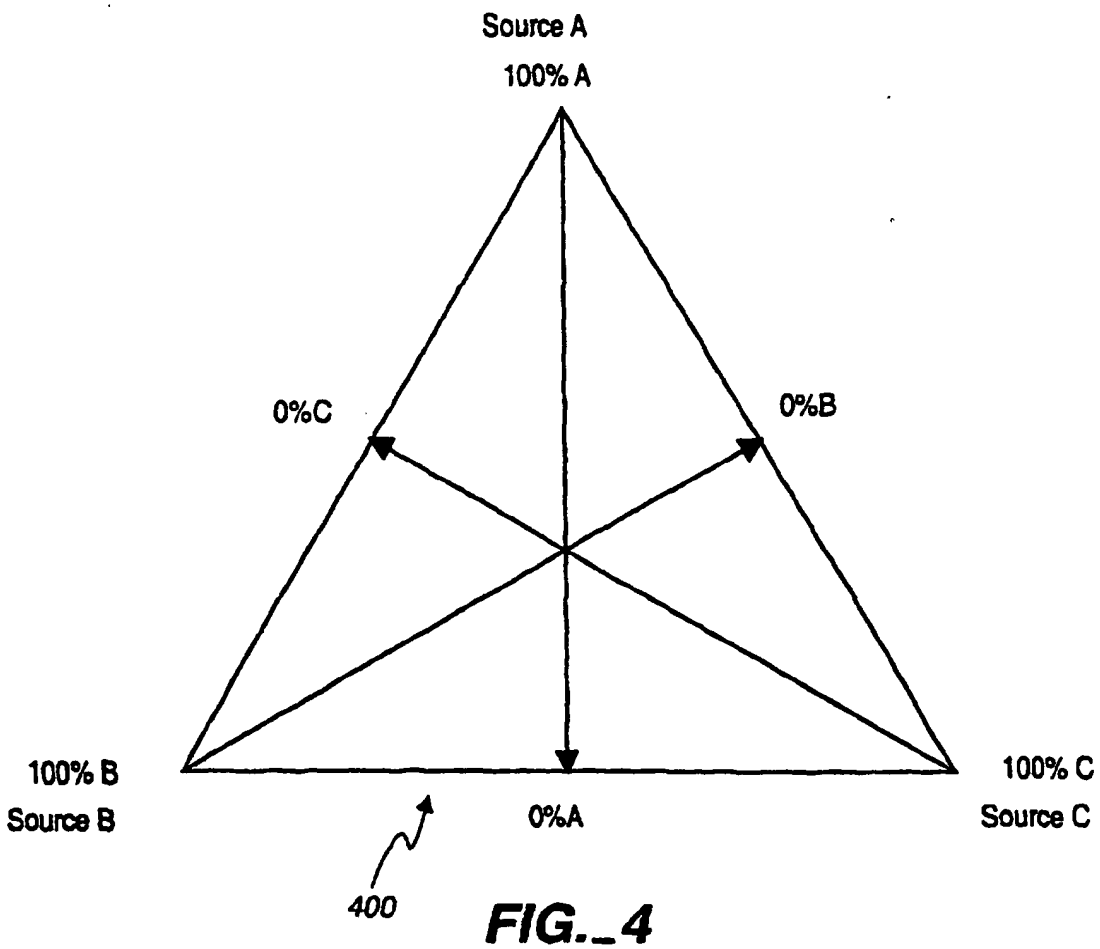

Source A
100% A
0%C
0%B
100% B
Source B
0%A
100% C
Source C
400

FIG._4

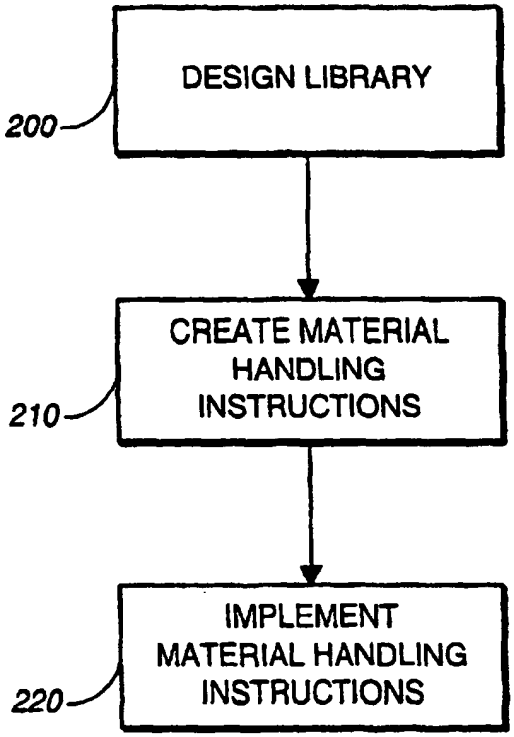

DESIGN LIBRARY
200
CREATE MATERIAL HANDLING INSTRUCTIONS
210
IMPLEMENT MATERIAL HANDLING INSTRUCTIONS
220

FIG._2

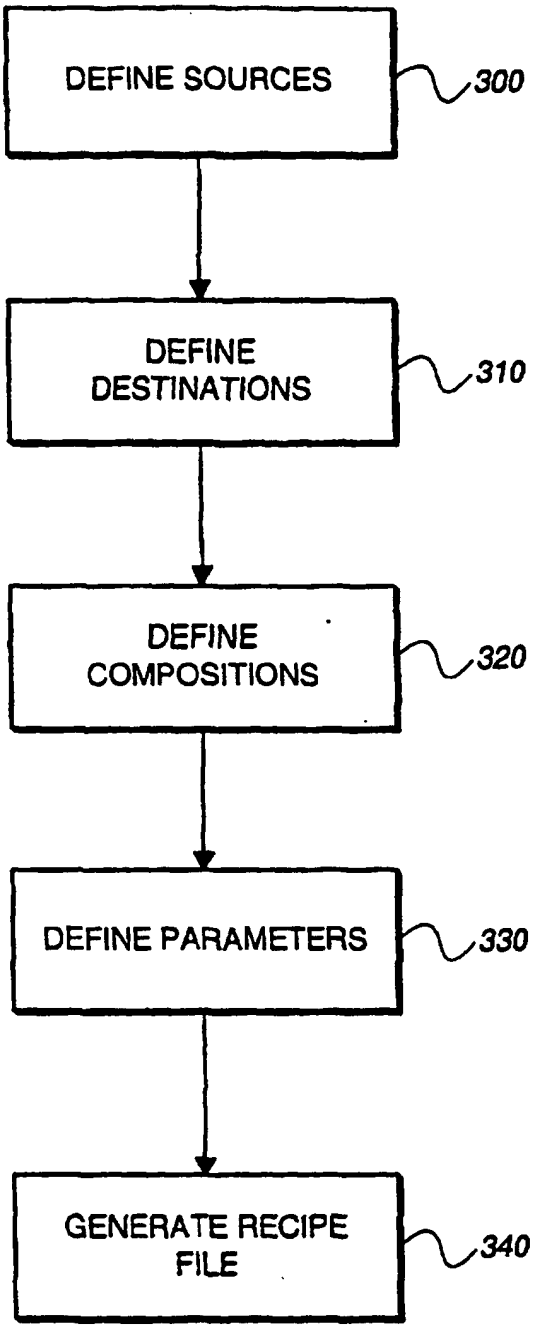

DEFINE SOURCES
300
DEFINE DESTINATIONS
310
DEFINE COMPOSITIONS
320
DEFINE PARAMETERS
330
GENERATE RECIPE FILE
340

FIG._3

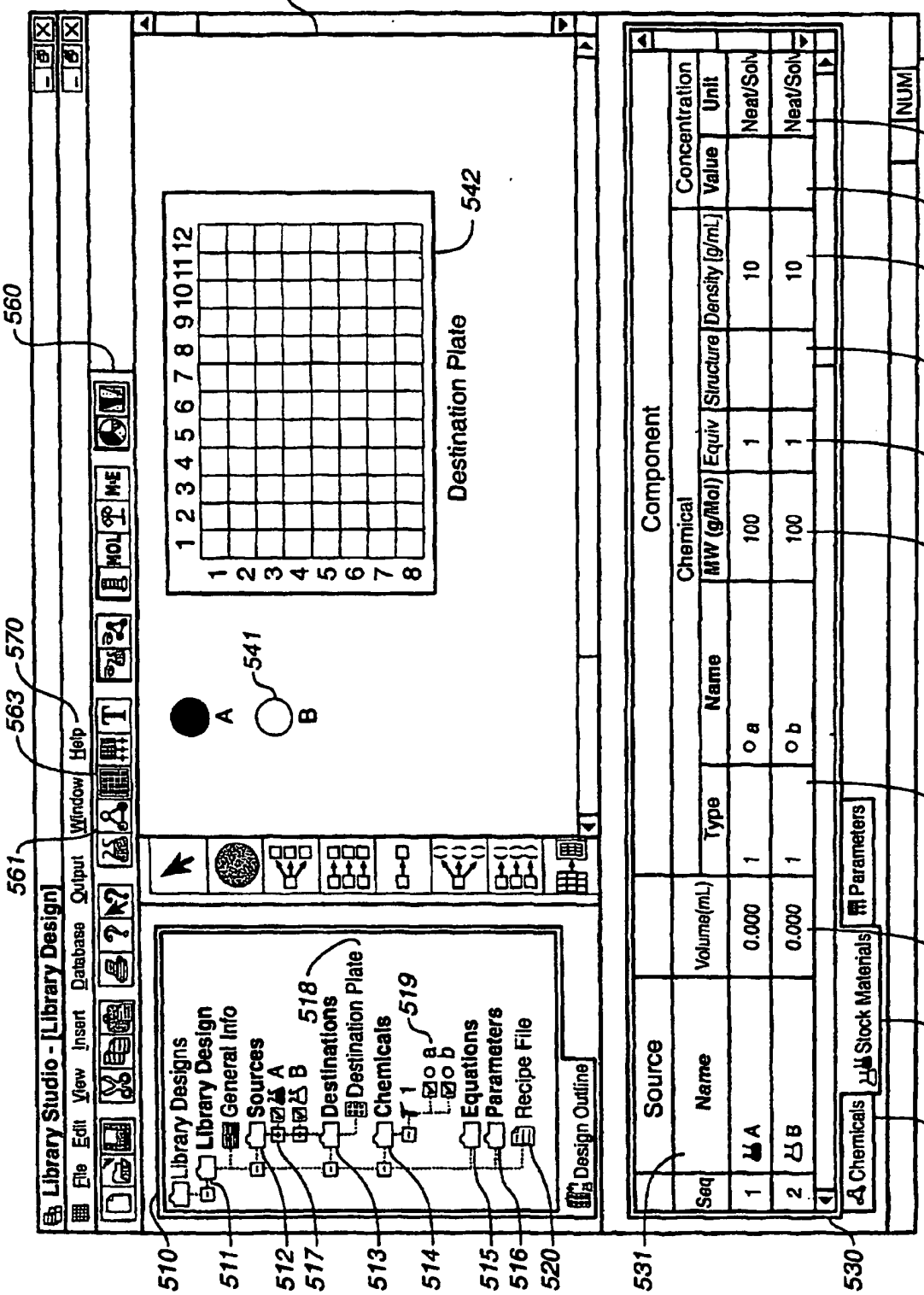

Library Studio - [Library Design]
File Edit View Insert Database Output Window Help
Library Designs
Library Design
General Info
Sources
A
B
Destinations
Destination Plate
Chemicals
1
a
b
Equations
Parameters
Recipe File
Design Outline
A
B
1 2 3 4 5 6 7 8 9 10 11 12
1 2 3 4 5 6 7 8
Destination Plate
Component
Source
Chemical
Concentration
Seq
Name
Volume(mL)
Type
Name
MW (g/Mol)
Equiv
Structure
Density [g/mL]
Value
Unit
1 A 0.000 1 a 100 1 10 Neat/Sol
2 B 0.000 1 b 100 1 10 Neat/Sol
Chemicals
Stock Materials
Parameters
NUM
510
511
512
517
513
514
515
516
520
518
519
530
531
532
533
534
535
536
537
538
539
540
541
542
545
525
561
563
570
560
500

FIG._5A

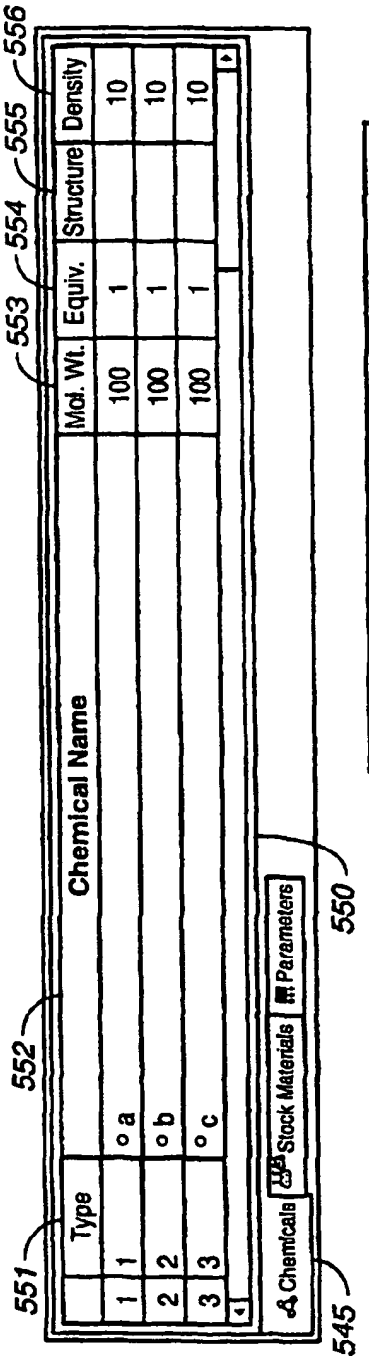

551
552
553
554
555
556
Type
Chemical Name
Mol. Wt.
Equiv.
Structure
Density
1 1 a 100 1 10
2 2 b 100 1 10
3 3 c 100 1 10
Chemicals
Stock Materials
Parameters
550
545

FIG._5B

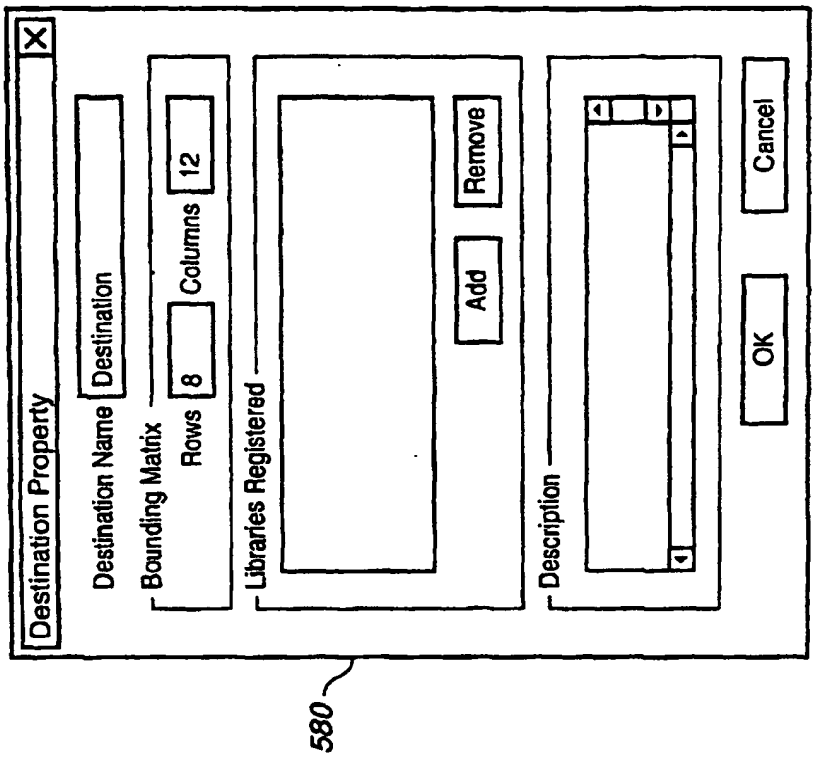

Destination Property
Destination Name
Destination
Bounding Matrix
Rows
8
Columns
12
Libraries Registered
Add
Remove
Description
OK
Cancel
580

FIG._5C

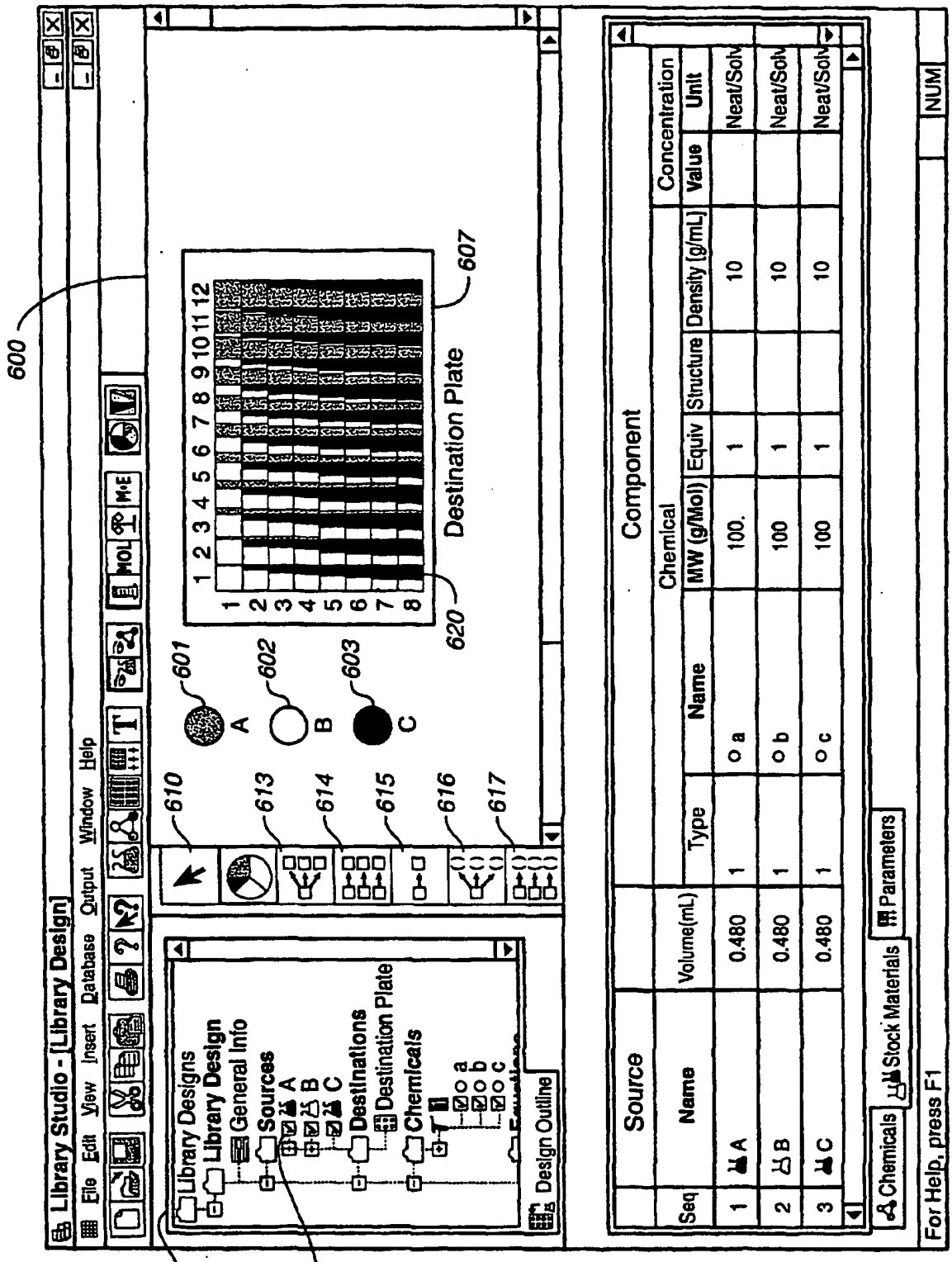

Library Studio - [Library Design]
File Edit View Insert Database Output Window Help
Library Designs
Library Design
General Info
Sources
A
B
C
Destinations
Destination Plate
Chemicals
a
b
c
Design Outline
1 2 3 4 5 6 7 8 9 10 11 12
1
2
3
4
5
6
7
8
Destination Plate
A
B
C
Source
Component
Chemical
Concentration
Seq
Name
Volume(mL)
Type
Name
MW (g/Mol)
Equiv
Structure
Density [g/mL]
Value
Unit
1 A 0.480 1 a 100. 1 10 Neat/Soln
2 B 0.480 1 b 100 1 10 Neat/Soln
3 C 0.480 1 c 100 1 10 Neat/Soln
Chemicals
Stock Materials
Parameters
For Help, press F1
NUM
600
601
602
603
607
610
613
614
615
616
617
620
670
675

FIG._6A

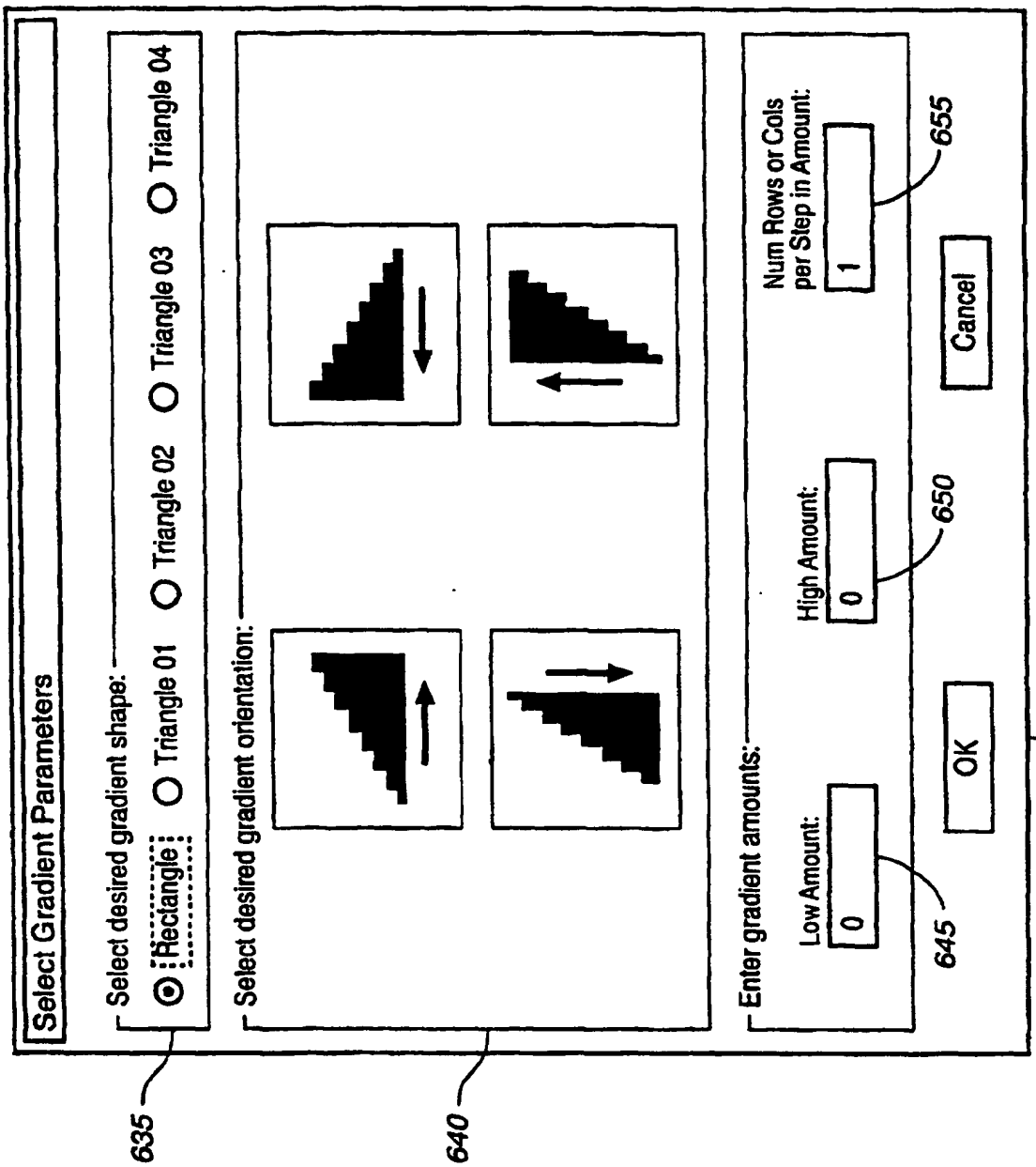

Select Gradient Parameters
Select desired gradient shape:
Rectangle
Triangle 01
Triangle 02
Triangle 03
Triangle 04
Select desired gradient orientation:
Enter gradient amounts:
Low Amount:
0
High Amount:
0
Num Rows or Cols per Step in Amount:
1
OK
Cancel
635
640
645
650
655
630

FIG._6B

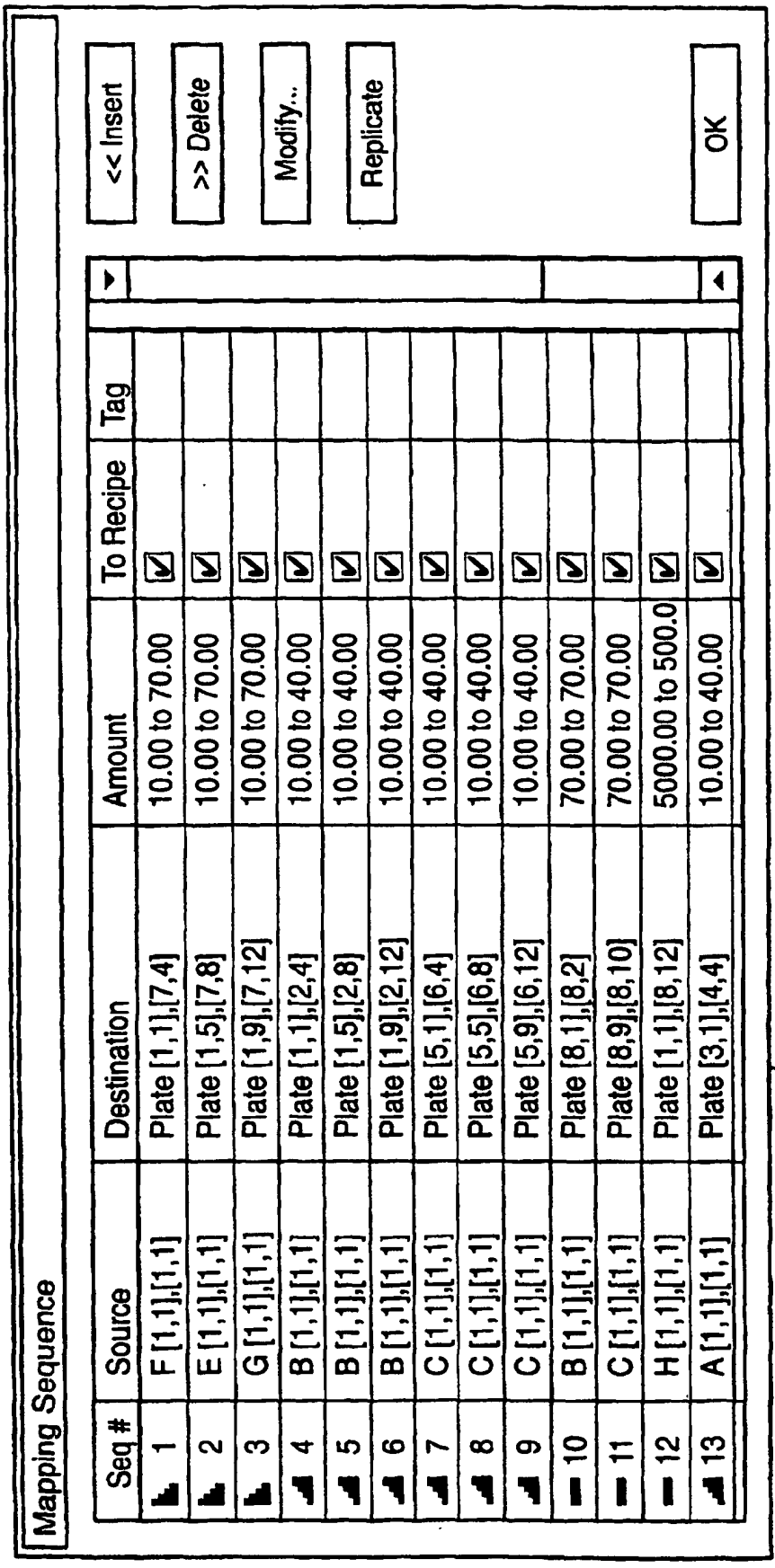

Mapping Sequence
Seq #
Source
Destination
Amount
To Recipe
Tag
1 F [1,1],[1,1] Plate [1,1],[7,4] 10.00 to 70.00
2 E [1,1],[1,1] Plate [1,5],[7,8] 10.00 to 70.00
3 G [1,1],[1,1] Plate [1,9],[7,12] 10.00 to 70.00
4 B [1,1],[1,1] Plate [1,1],[2,4] 10.00 to 40.00
5 B [1,1],[1,1] Plate [1,5],[2,8] 10.00 to 40.00
6 B [1,1],[1,1] Plate [1,9],[2,12] 10.00 to 40.00
7 C [1,1],[1,1] Plate [5,1],[6,4] 10.00 to 40.00
8 C [1,1],[1,1] Plate [5,5],[6,8] 10.00 to 40.00
9 C [1,1],[1,1] Plate [5,9],[6,12] 10.00 to 40.00
10 B [1,1],[1,1] Plate [8,1],[8,2] 70.00 to 70.00
11 C [1,1],[1,1] Plate [8,9],[8,10] 70.00 to 70.00
12 H [1,1],[1,1] Plate [1,1],[8,12] 5000.00 to 500.0
13 A [1,1],[1,1] Plate [3,1],[4,4] 10.00 to 40.00
<< Insert
>> Delete
Modify...
Replicate
OK
660

FIG._6C

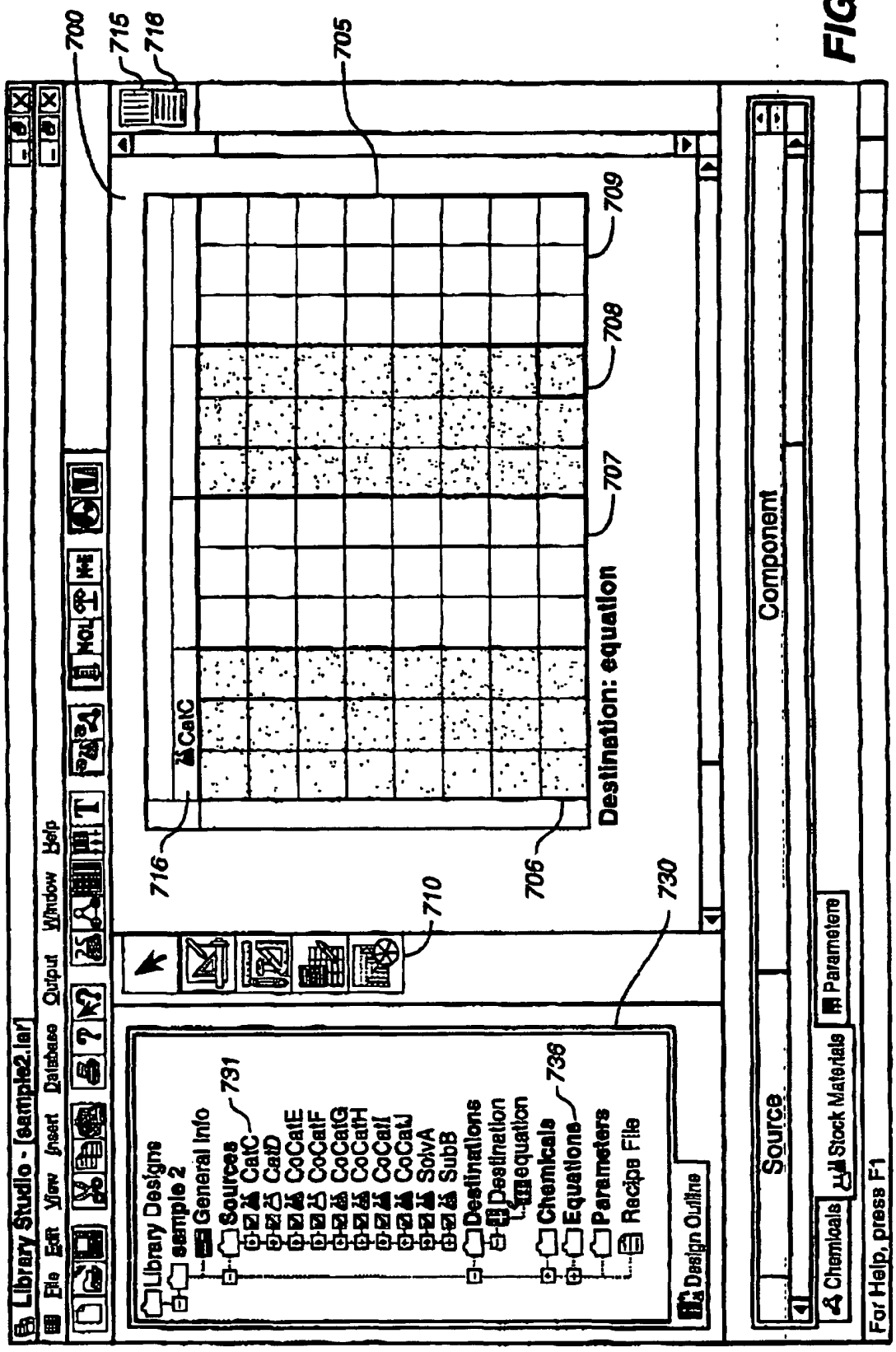

Library Studio - [sample2.lar]
File Edit View Insert Database Output Window Help
Library Designs
sample 2
General Info
Sources
CatC
CatD
CoCatE
CoCatF
CoCatG
CoCatH
CoCatI
CoCatJ
SolvA
SubB
Destinations
Destination
equation
Chemicals
Equations
Parameters
Recipe File
Design Outline
CatC
Destination: equation
Component
Source
Chemicals
Stock Materials
Parameters
For Help, press F1
700
715
716
705
709
708
707
706
710
730
731
736

FIG._7A

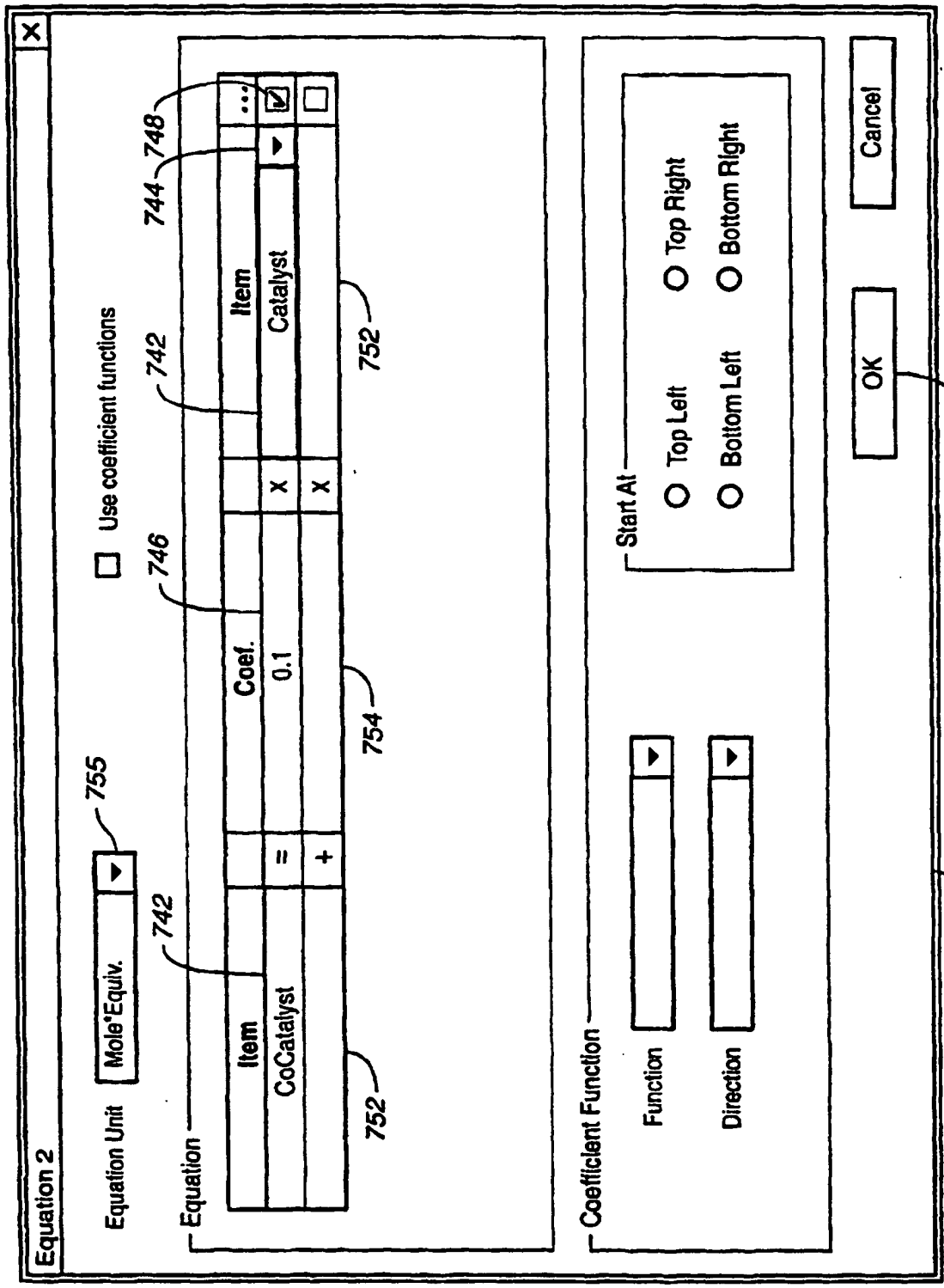

Equation 2
Equation Unit
Mole*Equiv.
755
Use coefficient functions
742
746
744
748
Equation
Item
Coef.
Item
...
CoCatalyst
=
0.1
x
Catalyst
+
x
752
754
752
Coefficient Function
Function
Direction
Start At
Top Left
Top Right
Bottom Left
Bottom Right
OK
Cancel
730
756

FIG._7B

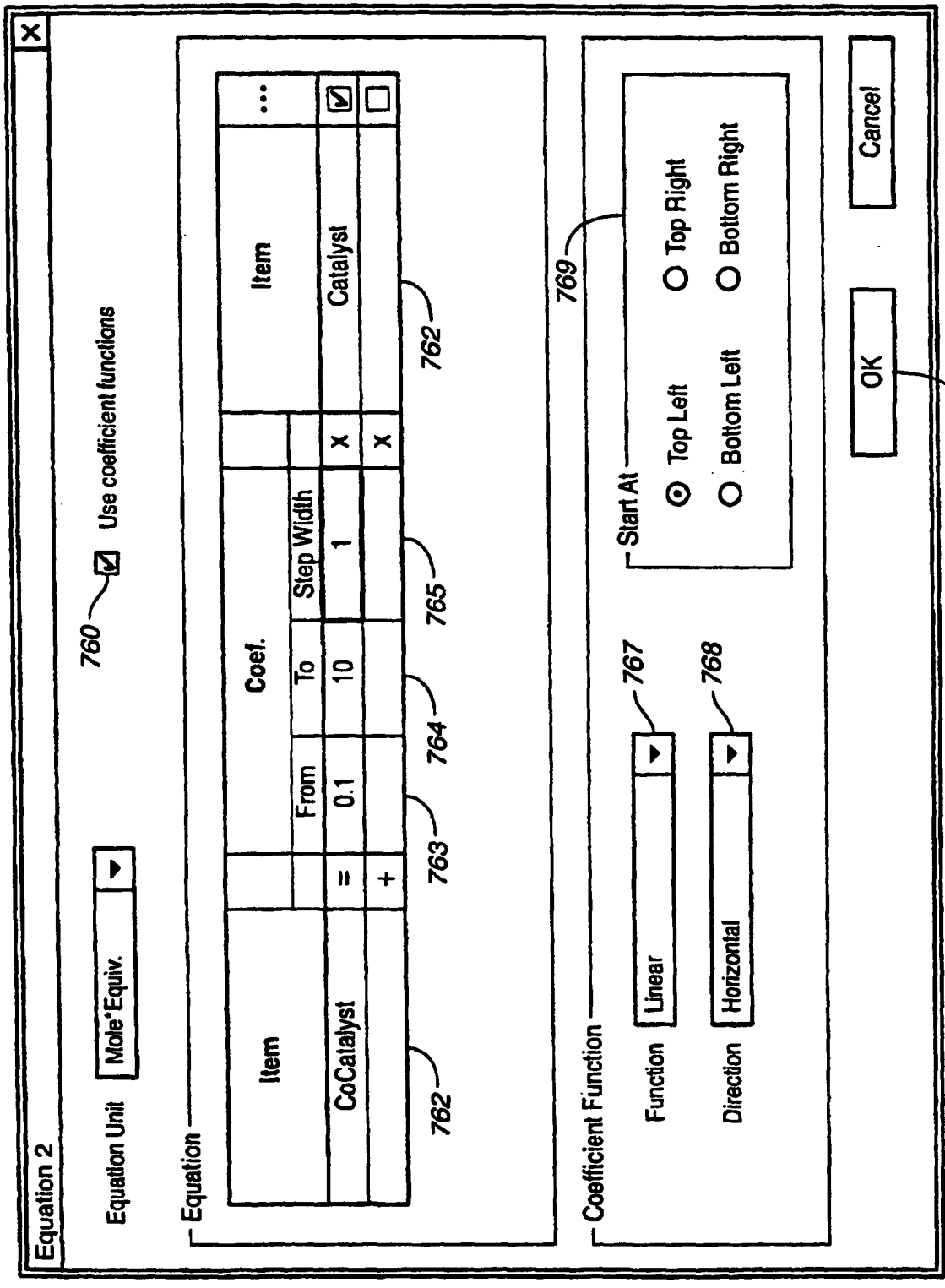

Equation 2
Equation Unit
Mole*Equiv.
760
Use coefficient functions
Equation
Item
Coef.
From
To
Step Width
Item
CoCatalyst
=
0.1
10
1
X
Catalyst
+
X
762
763
764
765
762
769
Coefficient Function
Function
Linear
767
Direction
Horizontal
768
Start At
Top Left
Top Right
Bottom Left
Bottom Right
OK
Cancel
770

FIG._7C

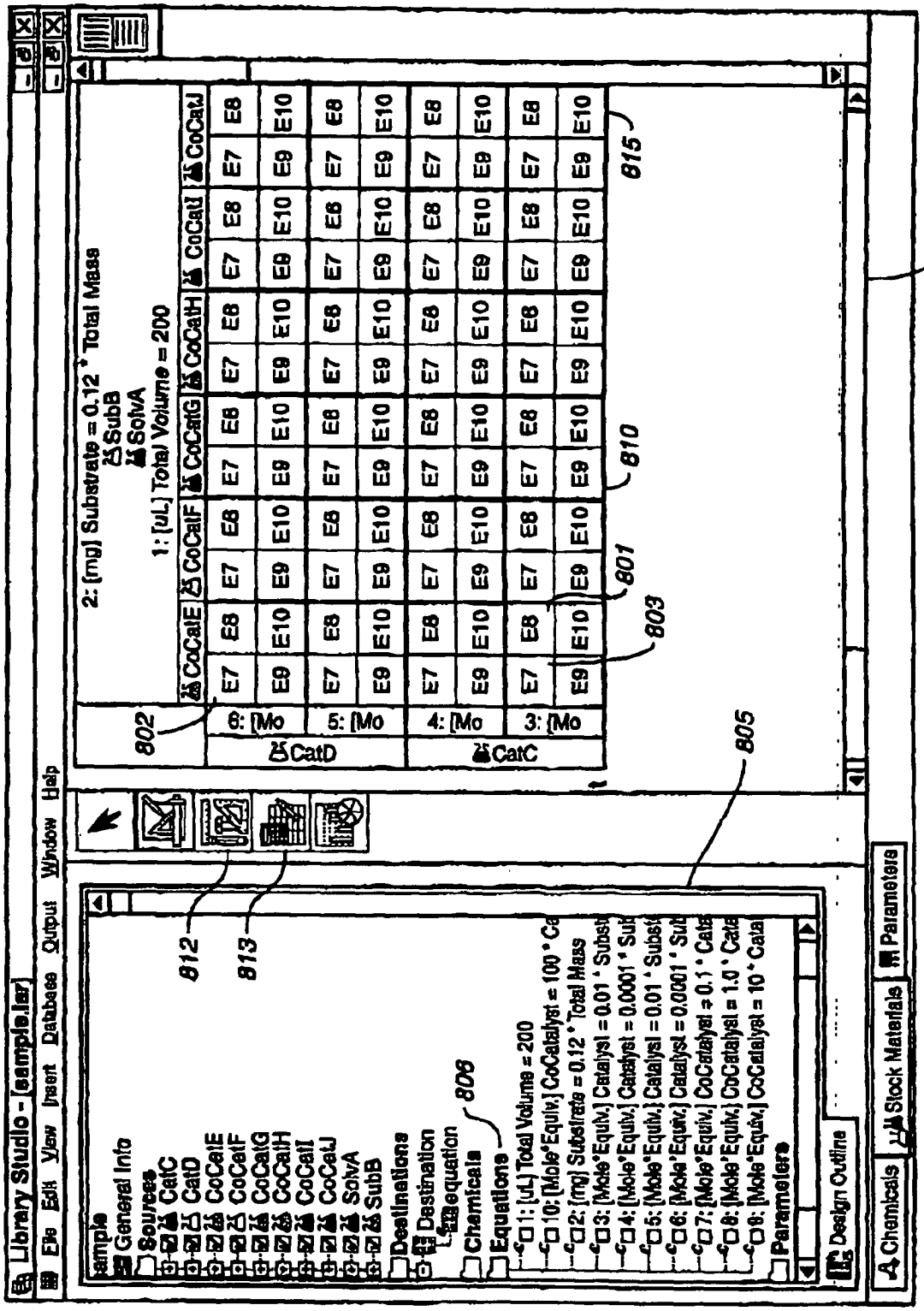
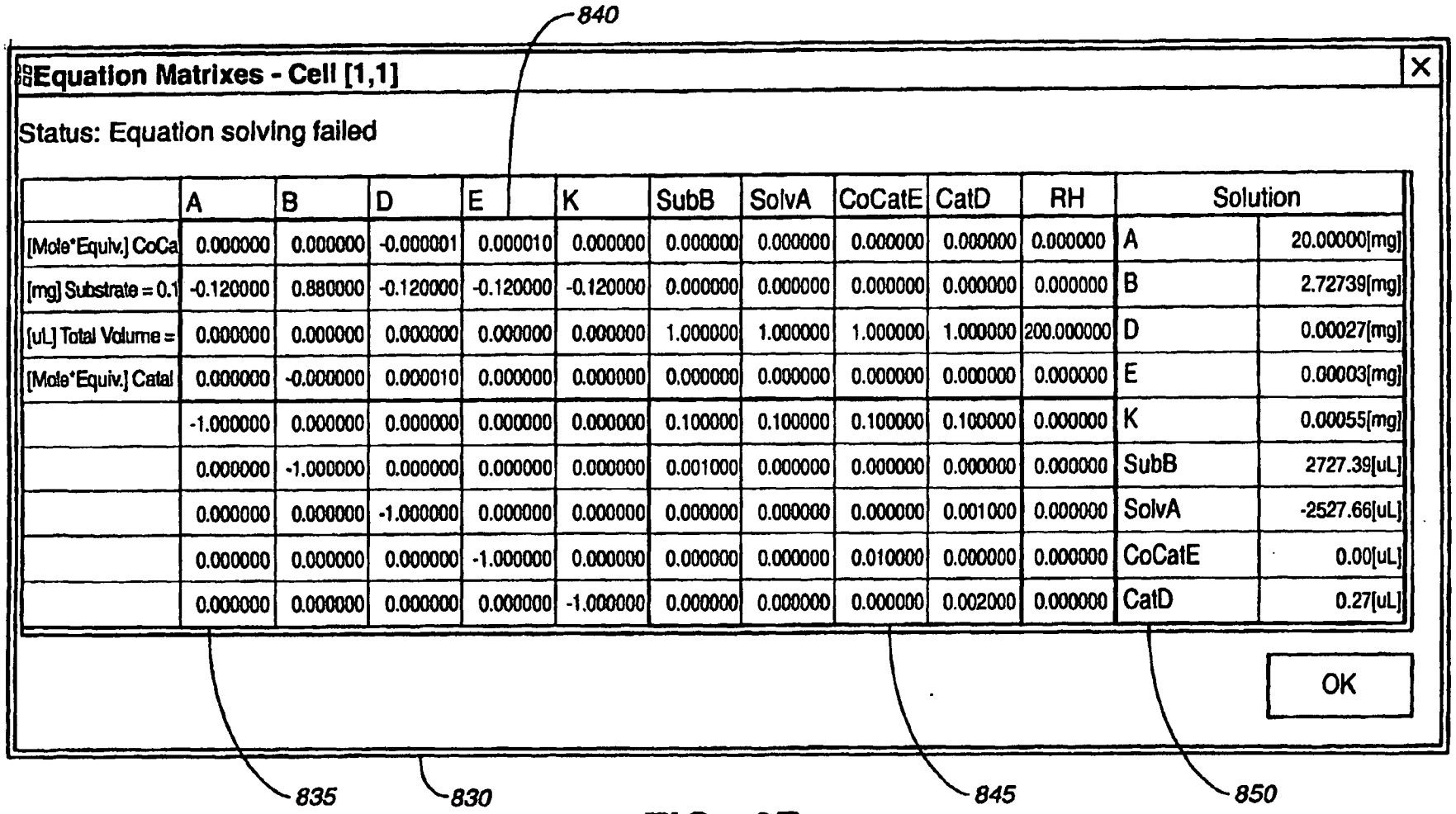

Library Studio - [sample.lar]
File Edit View Insert Database Output Window Help
sample
General Info
Sources
CatC
CatD
CoCatE
CoCatF
CoCatG
CoCatH
CoCatI
CoCatJ
SolvA
SubB
Destinations
Destination
Equation
Chemicals
Equations
1: [uL] Total Volume = 200
10: [Mole*Equiv.] CoCatalyst = 100 * Ca
2: [mg] Substrate = 0.12 * Total Mass
3: [Mole*Equiv.] Catalyst = 0.01 * Subst
4: [Mole*Equiv.] Catalyst = 0.0001 * Sub
5: [Mole*Equiv.] Catalyst = 0.01 * Subst
6: [Mole*Equiv.] Catalyst = 0.0001 * Sub
7: [Mole*Equiv.] CoCatalyst = 0.1 * Cata
8: [Mole*Equiv.] CoCatalyst = 1.0 * Cata
9: [Mole*Equiv.] CoCatalyst = 10 * Catal
Parameters
Design Outline
Chemicals
Stock Materials
Parameters
2: [mg] Substrate = 0.12 * Total Mass
SubB
SolvA
1: [uL] Total Volume = 200
CatD
CatC
6: [Mo
5: [Mo
4: [Mo
3: [Mo
812
813
802
801
803
805
806
810
815
800

FIG._8A




| | A | B | D | E | K | SubB | SolvA | CoCatE | CatD | RH | Solution | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| [Mole*Equiv.] CoCa | 0.000000 | 0.000000 | -0.000001 | 0.000010 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | A | 20.00000[mg] |
| [mg] Substrate = 0.1 | -0.120000 | 0.880000 | -0.120000 | -0.120000 | -0.120000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | B | 2.72739[mg] |
| [uL] Total Volume = | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 1.000000 | 1.000000 | 1.000000 | 1.000000 | 200.000000 | D | 0.00027[mg] |
| [Mole*Equiv.] Catal | 0.000000 | -0.000000 | 0.000010 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | E | 0.00003[mg] |
| | -1.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.100000 | 0.100000 | 0.100000 | 0.100000 | 0.000000 | K | 0.00055[mg] |
| | 0.000000 | -1.000000 | 0.000000 | 0.000000 | 0.000000 | 0.001000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | SubB | 2727.39[uL] |
| | 0.000000 | 0.000000 | -1.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.001000 | 0.000000 | SolvA | -2527.66[uL] |
| | 0.000000 | 0.000000 | 0.000000 | -1.000000 | 0.000000 | 0.000000 | 0.000000 | 0.010000 | 0.000000 | 0.000000 | CoCatE | 0.00[uL] |
| | 0.000000 | 0.000000 | 0.000000 | 0.000000 | -1.000000 | 0.000000 | 0.000000 | 0.000000 | 0.002000 | 0.000000 | CatD | 0.27[uL] |

FIG._8B

EP 1 080 435 B1

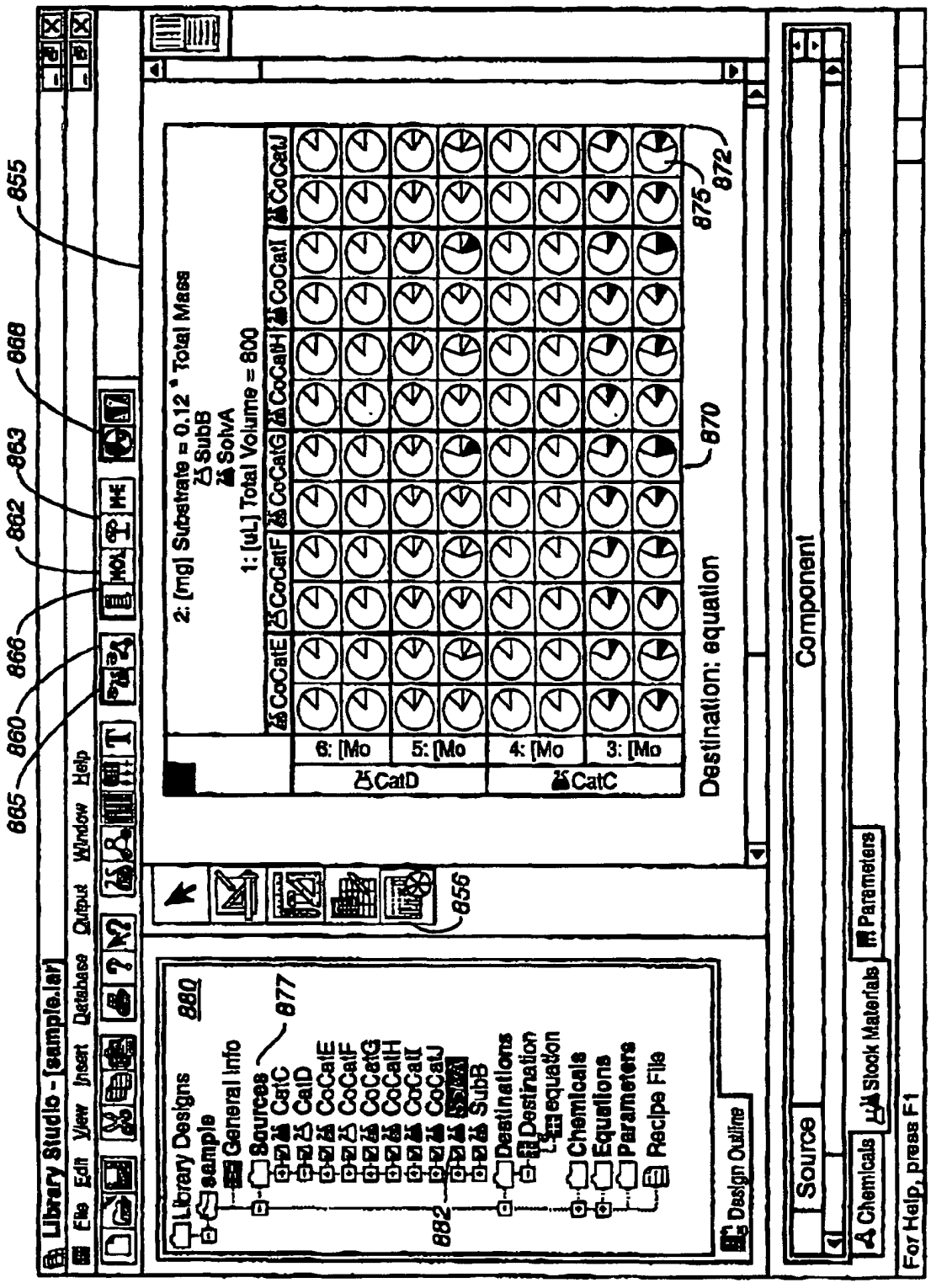

Library Studio - [sample.lar]
File Edit View Insert Database Output Window Help
Library Designs
sample
General Info
Sources
CatC
CatD
CoCatE
CoCatF
CoCatG
CoCatH
CoCatI
CoCatJ
SubB
Destinations
Destination
equation
Chemicals
Equations
Parameters
Recipe File
Design Outline
2: [mg] Substrate = 0.12 * Total Mass
SubB
SolvA
1: [uL] Total Volume = 800
CoCatE
CoCatF
CoCatG
CoCatH
CoCatI
CoCatJ
6: [Mo
5: [Mo
4: [Mo
3: [Mo
CatD
CatC
Destination: equation
Component
Source
Chemicals
Stock Materials
Parameters
For Help, press F1
855
856
860
862
863
866
868
870
872
875
877
880
882

FIG._8C

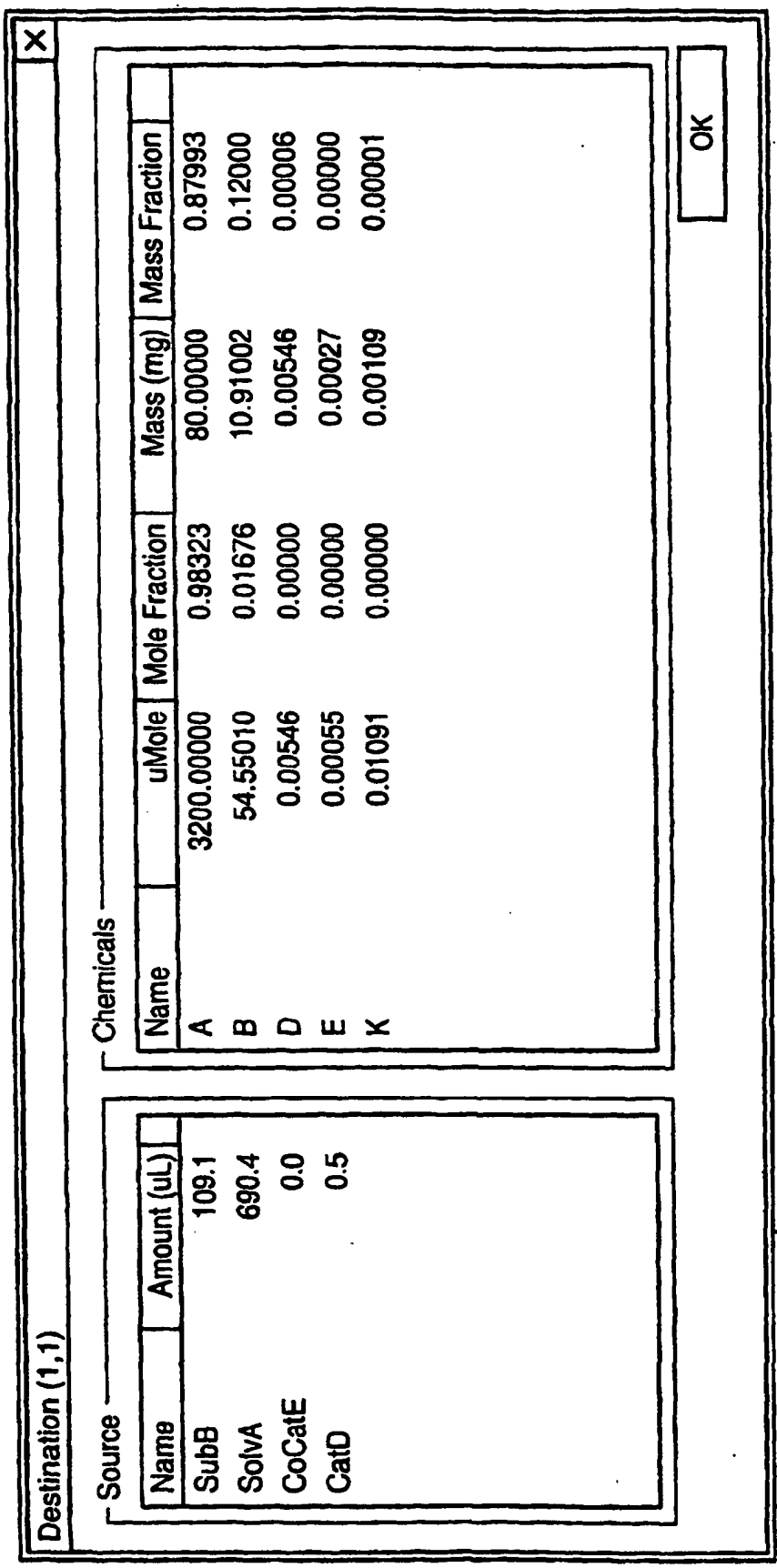

Destination (1,1)
Source
Name
Amount (uL)
SubB
109.1
SolvA
690.4
CoCatE
0.0
CatD
0.5
Chemicals
Name
uMole
Mole Fraction
Mass (mg)
Mass Fraction
A
3200.00000
0.98323
80.00000
0.87993
B
54.55010
0.01676
10.91002
0.12000
D
0.00546
0.00000
0.00546
0.00006
E
0.00055
0.00000
0.00027
0.00000
K
0.01091
0.00000
0.00109
0.00001
OK
885

FIG._8D

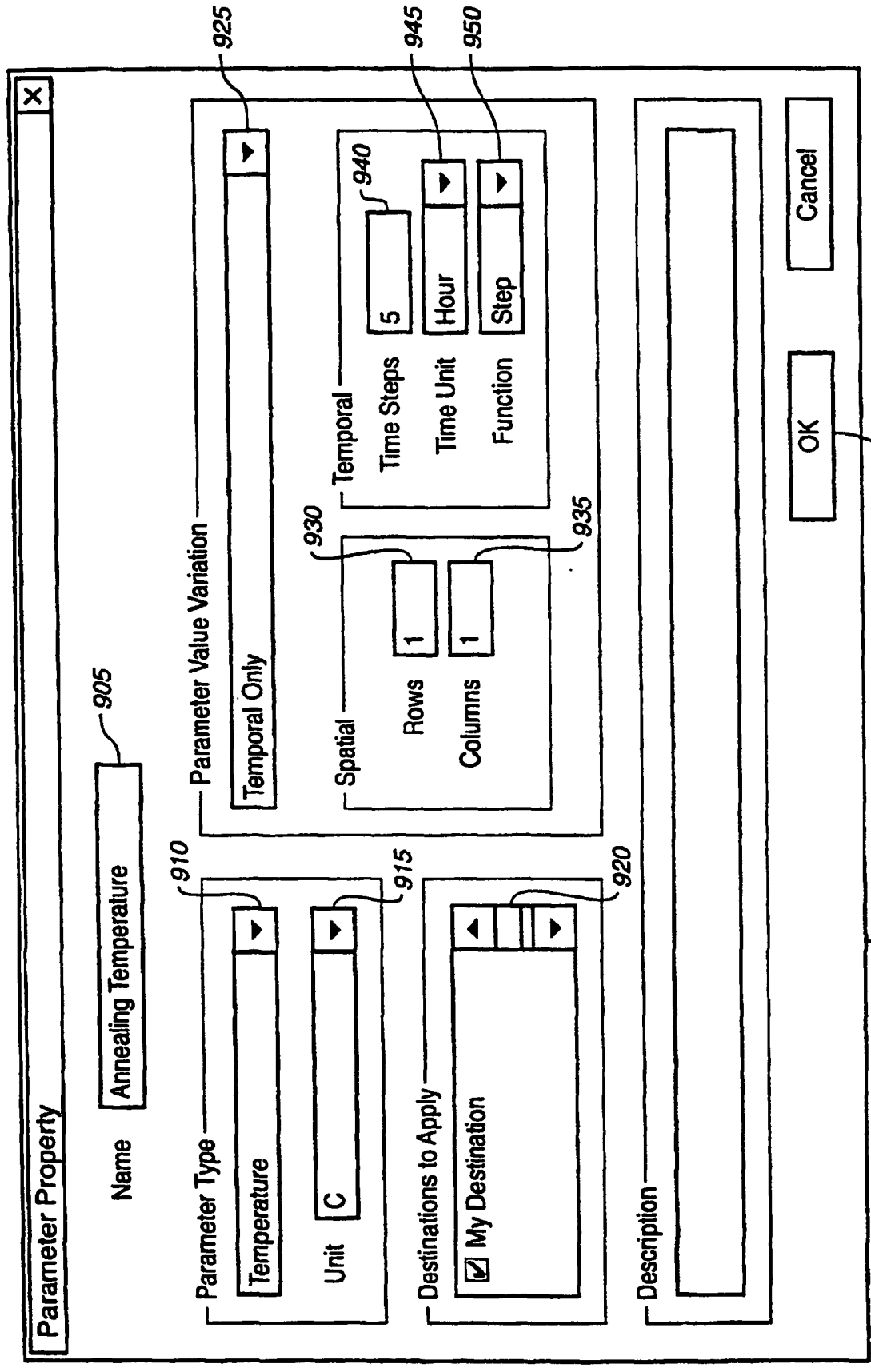

Parameter Property
Name
Annealing Temperature
905
Parameter Value Variation
925
Temporal Only
945
950
940
Temporal
Time Steps
5
Time Unit
Hour
Function
Step
930
935
Spatial
Rows
1
Columns
1
910
915
920
Parameter Type
Temperature
Unit
C
Destinations to Apply
My Destination
Description
OK
Cancel
960
900

FIG._9A

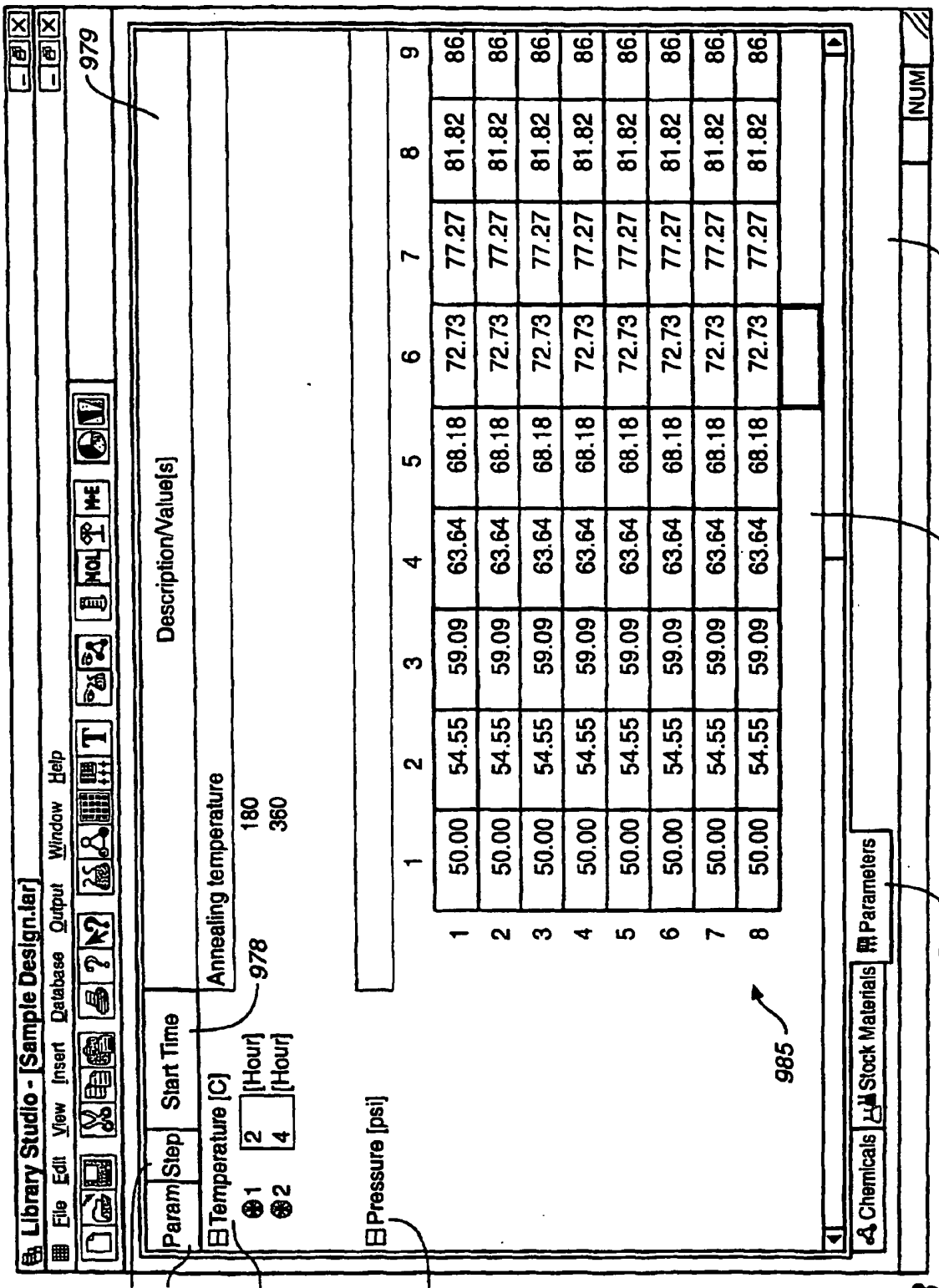

Library Studio - [Sample Design.lar]
File Edit View Insert Database Output Window Help
Param
Step
Start Time
Description/Value[s]
Temperature [C]
Annealing temperature
1
2
[Hour]
180
[Hour]
360
Pressure [psi]
1 2 3 4 5 6 7 8 9
1 50.00 54.55 59.09 63.64 68.18 72.73 77.27 81.82 86.
2 50.00 54.55 59.09 63.64 68.18 72.73 77.27 81.82 86.
3 50.00 54.55 59.09 63.64 68.18 72.73 77.27 81.82 86.
4 50.00 54.55 59.09 63.64 68.18 72.73 77.27 81.82 86.
5 50.00 54.55 59.09 63.64 68.18 72.73 77.27 81.82 86.
6 50.00 54.55 59.09 63.64 68.18 72.73 77.27 81.82 86.
7 50.00 54.55 59.09 63.64 68.18 72.73 77.27 81.82 86.
8 50.00 54.55 59.09 63.64 68.18 72.73 77.27 81.82 86.
Chemicals
Stock Materials
Parameters
NUM
977
976
975
980
978
979
985
970
965
968

FIG._9B

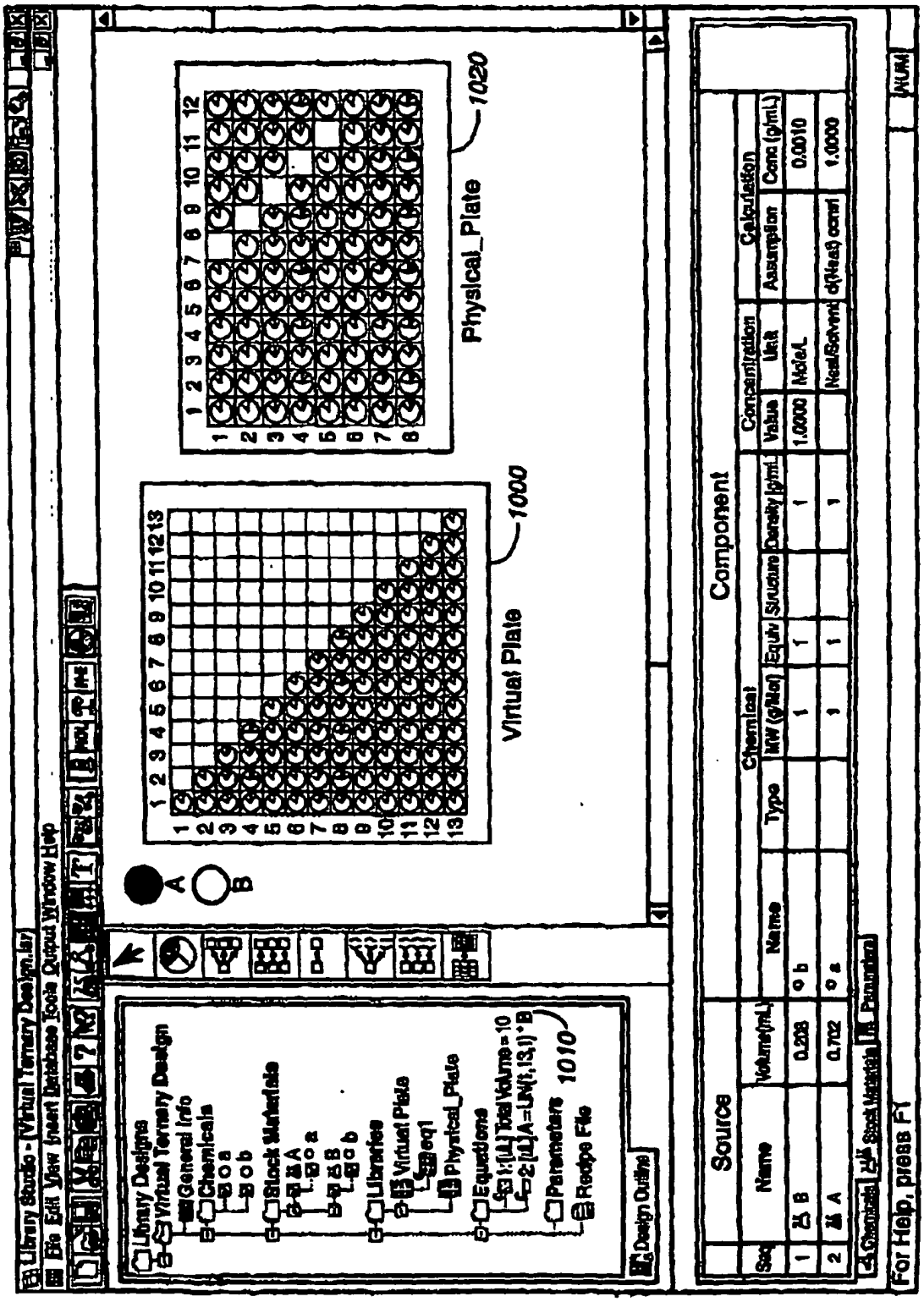

Physical_Plate
1020
Virtual Plate
1000
1010
Component
Source
Chemical
Concentration
Calculation
Seq
Name
Volume(mL)
Name
Type
MW (g/Mol)
Equiv
Structure
Density (g/mL)
Value
Unit
Assumption
Conc (g/mL)
1
B
0.208
b
1
1
1.0000
Mole/L
0.0010
2
A
0.702
a
1
1
1
Neat/Solvent
d(Neat) const
1.0000
For Help, press F1

FIG._10

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